STIC-EIC1600/2900

2565/2

Stom: Sent

CRAIG RICCI [craig root@usprc.gov] Thursday, April 03, 2008 3,23 PM STIO-E10 1508/2560

13: Cot.

NPI Emmoback

Subject:

Database Search Request Serial Number 10596911

Requestor: CRAIG RICGI (P/1914) Act was subjust ART USI JUST Fires. 3003

\$3.20 A D man

3864

Mailbox Number:

Case serial number: 10506911 Clies / Subcless(es): 514/383

Earliest Priority Filips Date: 102(b)=8/09/2004, 102(a.e)=0/12/2000

Former preferred for results: Paper

Attachment: No.

Search Topic Tabormation:

This is a follow up to a vestor request posted yestories for the same application. In most detail: Please search of Aim 1. Specifically, is there value art that renders any 1 or more of the alternative numbers of the group of stole derivatives of formula I (is, farmula I wherein A is 0, 8 is 0.8 is 0, 8 is 0, etc and hypernavely Also, if no gride art can be found to render 1 one more of the allernative members of the group of accis derivatives of lormals I not havel, our you please provide the following amplysis: 1. Do the expla derivatives of formula I se provided in which I have a common property or antivity? AND 2. Do they shake a common structure OF he they belong to a recognized class of chemical compounds in the art (in other words, can each remore be substituted for the other to provide the wank expected result?

apecial instructions and Other Comments:

Thank you.

A ALEXANDER OF THE STATE OF THE ACTIONS Secretary Footes Dato sekenek ingan ing Service Trop Cirts
Dating Trop

75.50 (2.50 2826 43, 2021.00 Seri Circonsi George Practi Stratite Practical Company Circonsi value exclusion deservations continue \$7%; W \$17%; 98 4.655 (146 147) 286-285 (146 147) 80908013 188779 888018188867 70900 1880888

=> file registry

FILE 'REGISTRY' ENTERED AT 14:24:28 ON 16 APR 2008 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file

provided by InfoChem.

STRUCTURE FILE UPDATES: 15 APR 2008 HIGHEST RN 1015083-77-8 DICTIONARY FILE UPDATES: 15 APR 2008 HIGHEST RN 1015083-77-8

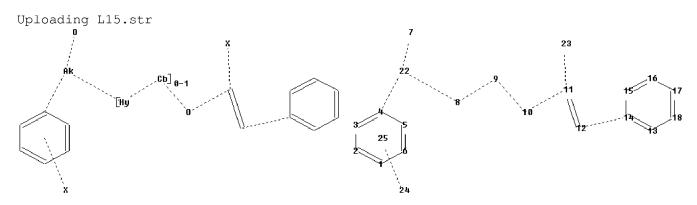
New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

# http://www.cas.org/support/stngen/stndoc/properties.html



```
chain nodes :
7  8  9  10  11  12  22  23  24
ring nodes :
1  2  3  4  5  6  13  14  15  16  17  18
chain bonds :
4-22  7-22  8-9  8-22  9-10  10-11  11-12  11-23  12-14
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  13-14  13-18  14-15  15-16  16-17  17-18
exact/norm bonds :
4-22  7-22  8-9  8-22  9-10  10-11  11-23  12-14
exact bonds :
11-12
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  13-14  13-18  14-15  15-16  16-17  17-18
```

# Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 22:CLASS 23:CLASS 24:CLASS 25:CLASS Generic attributes:

9:

Saturation : Unsaturated

Element Count : Node 8: Limited

N,N1

```
Uploading L45.str
                                                   31* "
Ну* <sup>2</sup>
                                                31* <sup>2</sup>
                                                                                    21
                           .cb] <sub>0-1</sub>
                                                                                     38
chain nodes :
7 8 9 10 11 12 21 22 24 27 30 31 36 38
ring nodes :
1 2 3 4 5 6 13 14 15 16 17 18
chain bonds :
4-27 \quad 7-27 \quad 8-9 \quad 8-27 \quad 9-10 \quad 10-11 \quad 11-12 \quad 11-21 \quad 12-14 \quad 12-38 \quad 27-36
ring bonds :
1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 13-14 \quad 13-18 \quad 14-15 \quad 15-16 \quad 16-17 \quad 17-18
exact/norm bonds :
4-27 8-9 8-27 9-10 11-21 12-38 27-36
exact bonds :
7-27 10-11 11-12 12-14
normalized bonds :
1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 13-14 \quad 13-18 \quad 14-15 \quad 15-16 \quad 16-17 \quad 17-18
G1:[*1],[*2]
G2:H,CF3
Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 21:CLASS
22:CLASS 24:CLASS
25:CLASS 26:CLASS 27:Atom 30:CLASS 31:Atom 36:CLASS 38:CLASS
Generic attributes :
9:
Saturation
                         : Unsaturated
27:
Saturation
                          : Saturated
31:
Saturation
                          : Unsaturated
Element Count :
Node 8: Limited
    N,N2
    C,C3
Node 9: Limited
   C,C6
```

```
Node 31: Limited N,N3 C,C3
```

```
Uploading L59.str
                                              2:*
  н* '
ну* <sup>2</sup>
                                           28* 2
                                                                           19
                        Cb] <sub>0-1</sub>
                    `[Hy
chain nodes :
7 8 9 10 19 20 21 24 27 28 33 35
ring nodes :
1 2 3 4 5 6 11 12 13 14 15 16
chain bonds :
4-24 7-24 8-9 8-24 9-10 10-35 12-35 19-35 24-33
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16
exact/norm bonds :
4-24 8-9 8-24 9-10 10-35 12-35 19-35 24-33
exact bonds :
7-24
normalized bonds :
1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 11-12 \quad 11-16 \quad 12-13 \quad 13-14 \quad 14-15 \quad 15-16
G1:[*1],[*2]
G2:H,CF3
Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 19:Atom 20:Atom 21:Atom
22:CLASS 23:CLASS
24:Atom 27:CLASS 28:Atom 33:CLASS 35:CLASS
Generic attributes :
9:
Saturation
                       : Unsaturated
24:
Saturation
                       : Saturated
28:
Saturation
                       : Unsaturated
35:
Saturation
                      : Unsaturated
Element Count :
Node 8: Limited
```

```
10/566911
```

N, N2 C, C3

Node 9: Limited

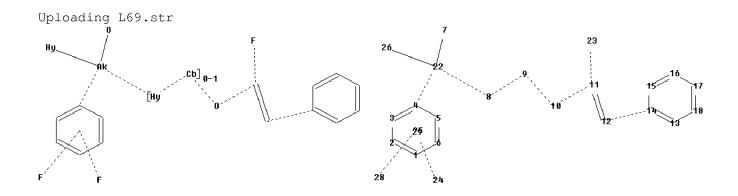
C,C6

Node 28: Limited

N, N3 C, C3

Node 35: Limited

C,C2-4



chain nodes :
7 8 9 10 11 12 22 23 24 26 28
ring nodes :
1 2 3 4 5 6 13 14 15 16 17 18
chain bonds :
4-22 7-22 8-9 8-22 9-10 10-11 11-12 11-23 12-14 22-26
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18
exact/norm bonds :
4-22 8-9 8-22 9-10 10-11 11-23 12-14 22-26
exact bonds :
7-22 11-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 22:CLASS 23:CLASS

25:CLASS 26:Atom 28:CLASS 29:CLASS

Generic attributes :

9:

Saturation : Unsaturated

Element Count : Node 8: Limited N,N1

Node 26: Limited N,N3 C,C3

=> file caplus FILE 'CAPLUS' ENTERED AT 14:24:31 ON 16 APR 2008 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 16 Apr 2008 VOL 148 ISS 16 FILE LAST UPDATED: 15 Apr 2008 (20080415/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

# http://www.cas.org/infopolicy.html 'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

=> d stat	que L	35				
L74	15476	SEA	FILE=CAPLUS	ABB=ON	PLU=ON	KIM B?/AU
L75	966	SEA	FILE=CAPLUS	ABB=ON	PLU=ON	MIN Y?/AU
L76	30107	SEA	FILE=CAPLUS	ABB=ON	PLU=ON	LEE Y?/AU
L77	1881	SEA	FILE=CAPLUS	ABB=ON	PLU=ON	PARK N?/AU
L78	9952	SEA	FILE=CAPLUS	ABB=ON	PLU=ON	KIM W?/AU
L79	1	SEA	FILE=CAPLUS	ABB=ON	PLU=ON	L74 AND L75 AND L76 AND L77
		AND	L78			
L80	13	SEA	FILE=CAPLUS	ABB=ON	PLU=ON	L74 AND L75 AND L76 AND L77
L81	1	SEA	FILE=CAPLUS	ABB=ON	PLU=ON	L74 AND L75 AND L76 AND L78
L82	1	SEA	FILE=CAPLUS	ABB=ON	PLU=ON	L74 AND L75 AND L77 AND L78
L83	1	SEA	FILE=CAPLUS	ABB=ON	PLU=ON	L74 AND L76 AND L77 AND L78
L84	1	SEA	FILE=CAPLUS	ABB=ON	PLU=ON	L75 AND L76 AND L77 AND L78
L85	13	SEA	FILE=CAPLUS	ABB=ON	PLU=ON	(L79 OR L80 OR L81 OR L82 OR
		L83	OR L84)			

#### => d ibib abs L85 1-13

L85 ANSWER 1 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2007:1453308 CAPLUS Full-text

DOCUMENT NUMBER: 148:55079

TITLE: Antifungal azole compounds capable of minimizing liver toxicity caused by long-term dosage and process for

toxicity caused by long-term dosage and process for

preparing the same

INVENTOR(S): Kim, Bum Tae; Min, Yong Ki; Heo, Jeong Nyung; Lee,

Hyuk; Lee, Woo Ghil; Kim, Soung Hwan; Park, No Kyun;

Lee, Yun Jeong; Kim, Hyoung Ho

PATENT ASSIGNEE(S): Korea Research Institute of Chemical Technology, S.

Korea

SOURCE: Repub. Korea, No pp. given

CODEN: KRXXFC

Patent DOCUMENT TYPE: LANGUAGE: Korean

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
KR 738228	B1	20070712	KR 2006-17423	20060222
PRIORITY APPLN. INFO.:			KR 2006-17423	20060222

AΒ Antifungal azole compds. and a process for preparing said compds. are claimed. Said compds. serve to improve antifungal activity, especially against fluconazole-resistant Candida albicans, and minimize liver toxicity caused by long-term dosage by enhancing safety of the compds. against the human Cytochrome P 450 enzyme. Antifungal triazole compds. (as represented by a certain formula; no data) or pharmaceutically acceptable salts or isomers thereof are claimed. Substituent groups in this formula may be selected from hydrogen, trifluoromethyl, etc., halo, C1-4 alkyl, C1-4 haloalkyl, C1-4 alkoxy, dioxymethylene group (incomplete list). Antifungal triazole compds. (as represented by a certain formula; no data) are prepared by treating alc. compds. (as represented by a certain formula; no data) with styrene compds. (as represented by a certain formula; no data) in the presence of base in organic solvent. More narrow definitions are indicated; however, specific chemical structures and/or addnl. information are not provided here.

L85 ANSWER 2 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN 2007:714281 CAPLUS Full-text ACCESSION NUMBER:

DOCUMENT NUMBER: 147:150765

Arylacrylates for the treatment of bone diseases TITLE: INVENTOR(S): Kim, Bum Tae; Min, Yong Ki; Lee, Yeon Soo; Heo,

Jung Nyoung; Lee, Hyuk; Park, No Kyun; Kim, Jung

Keun; Kim, Se Won; Ko, Seon Yle

PATENT ASSIGNEE(S): Korea Research Institute of Chemical Technology, S.

Korea; Oscotec Inc.

Repub. Korean Kongkae Taeho Kongbo, No pp. given SOURCE:

CODEN: KRXXA7

DOCUMENT TYPE: Patent LANGUAGE: Korean

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
KR 2006134303	А	20061228	KR 2005-53883	20050622
PRIORITY APPLN. INFO.:			KR 2005-53883	20050622

A pharmaceutical composition comprising an  $\alpha$ -arylmethoxy acrylate derivative AΒ is provided to be able to excellently inhibit osteoclast formation and absorption activity thereof, thereby being effectively utilized for preventing metabolic bone diseases such as osteoporosis and ossification at a growth period.

ACCESSION NUMBER: 2007:99425 CAPLUS Full-text

DOCUMENT NUMBER: 146:338005

TITLE: Process for easy preparation of a vinylphosphonate

having an  $\alpha\text{-tributyltin}$  group, used for

synthesis of organic phosphorous compounds

INVENTOR(S): Kim, Bum Tae; Min. Yong Ki; Lee, Yeon Soo; Heo,

Jung Nyoung; Lee, Hyuk; Lee, Woo Ghil; Kim, Seong

Hwan; Park, No Kyun; Heo, Yeon; Minami, Toru

PATENT ASSIGNEE(S): Korea Research Institute of Chemical Technology, S.

Korea

SOURCE: Repub. Korean Kongkae Taeho Kongbo, No pp. given

CODEN: KRXXA7

DOCUMENT TYPE: Patent LANGUAGE: Korean

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
KR 2006097214	A	20060914	KR 2005-18285	20050304
PRIORITY APPLN. INFO.:			KR 2005-18285	20050304

AB A method for preparing a vinylphosphonate having an  $\alpha$ -tributyltin group is provided to conveniently synthesize a vinylphosphonate by using reactivity of the tributyltin; the latter vinylphosphonate is then used for preparing various compds. To prepare a vinylphosphonate derivative, a vinylphosphonate having an  $\alpha$ -tributyltin group prepared by reacting acetylene phosphonate with tributyltin hydride in the presence of Pd catalyst and a solvent is reacted with a halide compound including an R group (R = C2-6 alkyl, aryl, heterocyclic compound such as pyridine, pyrimidine, thiophene, quinoline substituted by alkyl, alkoxy, and halogen) in the presence of Pd catalyst such as Pd(PPh3)4, PdCl2(PPh3)2, BnPdCl(PPh3)2 and Pd2dba3, an inorg. salt and a solvent selected from the group consisting of THF, DMF, N-methylpyrrolidinone, benzene, and toluene.

L85 ANSWER 4 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:960988 CAPLUS Full-text

DOCUMENT NUMBER: 145:470053

TITLE: Process for preparation of alkyl s-(1)-lactate and

alkyl r-(d)-o-acyllactate by using lipase which allows to improve preparation yield and optical purity, and

enhance separation convenience of product

INVENTOR(S): Lee, Yeon Soo; Kim, Bum Tae; Min, Yong Ki; Heo,

Jung Nyoung; Lee, Woo Ghil; Park, No Kyun

oung Nyoung, Lee, woo Gill, Laxx, No Myon

PATENT ASSIGNEE(S): Korea Research Institute of Chemical Technology, S.

Korea

SOURCE: Repub. Korean Kongkae Taeho Kongbo, No pp. given

CODEN: KRXXA7

DOCUMENT TYPE: Patent LANGUAGE: Korean

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
KR 2005103691	A	20051101	KR 2004-28968	20040427
PRIORITY APPLN. INFO.:			KR 2004-28968	20040427

AB A process for preparation of alkyl S-(L)-lactate and alkyl R-(D)-O-acyllactate by using lipase is provided to improve the preparation yield and optical

purity, and enhance the separation convenience of the product. The process for preparation of alkyl S-(L)-lactate of formula (2) and alkyl R-(D)-O-acyllactate of formula (3) comprises reacting racemic alkyl lactate of formula (1) in the presence of lipase with carbonyl donor at 0 to 80° for 1 to 100 h to stereoselectively carbonylate a hydroxide group of alkyl R-lactate, wherein R is C1-C10 of saturated or unsatd. alkyl, or alkyl substituted aryl or heteroaryl; R1 is C1-C10 of saturated or unsatd. alkyl, or aryl; and the lipase is derived from Candida antarctica.

L85 ANSWER 5 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2006:841833 CAPLUS Full-text

DOCUMENT NUMBER: 145:241781

TITLE: Compositions comprising methoxyacrylate-based

compounds for the treatment of osteoporosis

INVENTOR(S): Kim, Bam Tae; Kim, Ho Soon; Kim, Jung Keun; Kim,

Jung Yeo; Kim, Se Won; Ko, Seon Yle; Lee, Byung Eui; Lee, Yeon Soo; Min, Yong Ki; Oh, Kwi Ok; Park, No Kyun

PATENT ASSIGNEE(S): Korea Research Institute of Chemical Technology, S.

Korea; Oscotec Inc.

SOURCE: Repub. Korean Kongkae Taeho Kongbo, No pp. given

CODEN: KRXXA7

DOCUMENT TYPE: Patent LANGUAGE: Korean

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
KR 2005002109	A	20050107	KR 2003-43425	20030630
PRIORITY APPLN. INFO.:			KR 2003-43425	20030630

AB The composition inhibits osteoclast generation and bone absorption without cytotoxicity to prevent or treat osteoporosis. The pharmaceutical composition for prevention and treatment of osteoporosis is characterized by containing as an active ingredient, a methoxyacrylate-based compd pharmaceutically acceptable carriers.

L85 ANSWER 6 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2006:721491 CAPLUS Full-text

DOCUMENT NUMBER: 145:118712

TITLE: Propenoic ester and amide derivatives having

fluorostyrene substituent, process for preparing the same and antifungal composition comprising the same

INVENTOR(S): Kim, Beom Tae; Kim, Jin Cheol; Lee, Yeon Su; Min,

Yong Gi; Park, No Gyun

PATENT ASSIGNEE(S): Korea Research Institute of Chemical Technology, S.

Korea

SOURCE: Repub. Korean Kongkae Taeho Kongbo, No pp. given

CODEN: KRXXA7

DOCUMENT TYPE: Patent LANGUAGE: Korean

FAMILY ACC. NUM. COUNT: 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
KR 2004067218	А	20040730	KR 2003-4230	20030122
PRIORITY APPLN. INFO.:			KR 2003-4230	20030122

AΒ Propenoic ester and amide derivs. having a fluorostyrene substituent, a process for preparing the same compds. and an antifungal composition comprising the same compds. are provided, which have improved antifungal activity at a low concentration, wide range of antifungal activity, low toxicity and improved duration of efficacy. The process for preparing the propenoic ester and amide derivs. comprises the steps of: reacting a bromide compound with 3-hydroxybenzaldehyde in the presence of base; and Wittig reacting the compound to prepare propenoic ester.

L85 ANSWER 7 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN 2005:1350944 CAPLUS Full-text ACCESSION NUMBER:

DOCUMENT NUMBER: 144:88045

Preparation of  $\alpha$ -arylmethoxyacrylates for use in TITLE:

pharmaceutical compositions for preventing and

treating metabolic bone diseases

Kim, Bum Tae; Min, Yong Ki; Lee, Yeon Soo; Heo, INVENTOR(S):

Jung Nyoung; Lee, Hyuk; Park, No Kyun; Kim,

Jung-Keun; Kim, Se-Won; Ko, Seon-Yle

PATENT ASSIGNEE(S): Korea Research Institute of Chemical Technology, S.

Korea: Oscotec Inc.

PCT Int. Appl., 74 pp. SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PA'	PATENT NO.					KIND DATE			APPLICATION NO.							DATE			
WO	2005	1230	54		A1		2005	1229	,	WO 2	005-	KR19.	35		2	0050	622		
	W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,		
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,		
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KM,	ΚP,	KΖ,	LC,		
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NG,		
		NΙ,	NO,	NΖ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,		
		SM,	SY,	ΤJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,		
		ZM,	ZW																
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,		
		ΑZ,	BY,	KG,	KΖ,	MD,	RU,	ΤJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,		
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,	IS,	ΙΤ,	LT,	LU,	MC,	NL,	PL,	PT,		
		RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,		
		MR,	NE,	SN,	TD,	ΤG													
KR	2005	1214	91		Α	A 20051227				KR 2004-46644						20040622			
EP	1784	173			A1		2007	0516		EP 2	005-	7568	53		2	0050	622		
	R:	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,		
			•	•	•			NL,		•	•		•	•					
	1968							0523											
	2008				Τ		2008	0207											
PRIORIT	ORITY APPLN. INFO.:			.:						KR 2	004-	4664	4		A 2	0040	622		
											005-				W 2	0050	622		
OTHER SO	DURCE	(S):			CASI	REAC	T 14	4:880	045;	MAR	PAT	144:	8804	5					

$$\begin{array}{c} X \\ \\ MeO \end{array} \begin{array}{c} X \\ Y \end{array} \begin{array}{c} A \\ \\ Z \end{array} \begin{array}{c} R1 \end{array}$$

AB The title compds. I [A = 0, S, CH2, ON:CH, ON:C(Me); X = H, halo; Y = N, CH; Z = 0, NH; R1 = H, alkyl; R2 = (un)substituted (hetero)aryl], useful for preventing and treating metabolic bone diseases, were prepared and disclosed. E.g., a multi-step synthesis of (E)-Me  $2-(2-\{[4-(cyclopropylmethyl)phenoxy]methyl\}-4-chlorophenyl)-3-methoxyacrylate (II), starting from 2-bromo-5-chlorotoluene, was given. II showed 100% inhibition of osteoclast formation at 1.0 <math>\mu$ M.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L85 ANSWER 8 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2005:141060 CAPLUS Full-text

DOCUMENT NUMBER: 142:240437

TITLE: Preparation of triazolylmethanol derivatives as

antifungal agents

INVENTOR(S): Kim, Bum Tae; Min, Yong Ki; Lee, Yeon Soo;

Park, No Kyun; Kim, Woo Jung

PATENT ASSIGNEE(S): Korea Research Institute of Chemical Technology, S.

Korea

SOURCE: PCT Int. Appl., 58 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

	PATENT NO.						KIND DATE			-	APPL	ICAT		DATE				
	WO	2005	0145	83		A1	_	2005	0217	,	WO 2	004-	KR19		20040809			
		W:	ΑE,	ΑG,	AL,	AM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
			CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
			GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KP,	KΖ,	LC,	LK,
			LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,	NO,
			NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	ТJ,
			TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW	
		RW:	BW,	GH,	GM,	ΚE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,
			ΑZ,	BY,	KG,	KΖ,	MD,	RU,	ΤJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
			EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	IT,	LU,	MC,	NL,	PL,	PT,	RO,	SE,
			SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	ΝE,
			SN,	TD,	ΤG													
	KR	2005	0179	62		Α		2005	0223		KR 2	003-	5559	20030812			812	
	ΕP	1654	254			A1		2006	0510		EP 2	004-	7485.	24		2	0040	809
		R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙΤ,	LI,	LU,	NL,	SE,	MC,	PT,
			ΙE,	SI,	FI,	RO,	CY,	TR,	BG,	CZ,	EE,	HU,	PL,	SK				
	JΡ	2007	5022	68		Τ		2007	0208	1	JP 2	006-	5231.	25		2	0040	809
	US	2008	0027	117		A1		2008	0131	US 2006-566911					20060203			
PRIO	PRIORITY APPLN. INFO.:				.:						KR 2	003-	5559	0	Ĩ	A 2	0030	812

WO 2004-KR1996 W 20040809

OTHER SOURCE(S): CASREACT 142:240437; MARPAT 142:240437

Т

ΙI

GΙ

AB Title compds. represented by the formula I [wherein A = 0, 1,2,4-triazolyl-PhO-, 1,2,4-triazolone-3-yl-PhO-, imidazolone-1-yl-PhO, imidazolinone-1-yl-PhO-; R = H or CF3; R' = H or alkyl; X = H, halo, (halo)alkyl,alkoxy, 3,4-dioxyalkylene; and pharmaceutically acceptable salts, isomers or esters thereof] were prepared as antifungal agents for the treatment of humans or animals. For example, II was given in a multi-step synthesis starting from the reaction of Me (R)-lactate with morpholine. I showed antifungal activity in vivo against a wide spectrum of pathogenic fungi, such as ATCC 10231 and MYA-573, and low toxicity in oral administration.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L85 ANSWER 9 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2004:943976 CAPLUS Full-text

DOCUMENT NUMBER: 142:155964

TITLE: Method for preparation of fluorine-substituted

heterocyclic compounds as intermediate for synthesis

of agrochemical and medicinal antagonist

INVENTOR(S): Kim, Beom Tae; Lee, Yeon Su; Min, Yong Gi;

Park, No Gyun

PATENT ASSIGNEE(S): Korea Research Institute of Chemical Technology, S.

Korea

SOURCE: Repub. Korean Kongkae Taeho Kongbo, No pp. given

CODEN: KRXXA7

DOCUMENT TYPE: Patent LANGUAGE: Korean

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

KR 2003031795	A	20030423	KR 2001-63681	20011016
KR 2004043142	A	20040522	KR 2004-21097	20040329
PRIORITY APPLN. INFO.:			KR 2001-63681	A3 20011016

AB Provided are a fluorine-substituted heterocyclic compds., 5-fluoropyrazole derivative and 4-fluoro-6-hydroxypyrimidine, useful as intermediates for the synthesis of agrochems. and medicinal antagonists and methods for preparing them regio selectively in high yields. The fluorine-substituted heterocyclic compds., 5-fluorpyrazole derivative and 4-fluor-6-hydroxy pyrimidine are represented by the formula(1a) or(1b), and formula(2) resp., wherein X is hydrogen, halogen, C1-4 alkyl, C1-4 alkoxy or C1-C4 arylalkyloxy; RF is fluorine or trifluoromethyl; and R1, R2 and R3 are individually hydrogen, C1-4 alkyl, C1-4 aryl or C1-4 arylalkyl. They are manufactured by one pot reaction with a substituted hydrazine derivative and a guanidine derivative using Me 2-fluoralkyl 2-phenylacetate derivative as a starting material.

L85 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2004:923755 CAPLUS  $\underline{\text{Full-text}}$ 

DOCUMENT NUMBER: 142:113616

TITLE: Preparation of novel propanoic ester and amide

derivatives having oxime group as branched chain and

disinfectant composition containing the same

Kim, Beom Tae; Kim, Gyeong Man; Kim, Heung Tae;

Lee, Yeon Su; Min, Yong Gi; Park, No Gyun

PATENT ASSIGNEE(S): Korea Research Institute of Chemical Technology, S.

Korea

SOURCE: Repub. Korean Kongkae Taeho Kongbo, No pp. given

CODEN: KRXXA7

DOCUMENT TYPE: Patent LANGUAGE: Korean

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

INVENTOR(S):

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
KR 2002040158	A	20020530	KR 2000-70103	20001123
PRIORITY APPLN. INFO.:			KR 2000-70103	20001123

AB Provided are novel propanoic ester and amide derivs. having an oxime group as a branched chain, which are excellent in disinfecting activity, a preparation thereof, and a disinfectant composition containing the propanoic ester and amide derivs. The propanoic ester and amide derivs. represented by the formula 1 are produced by a process comprising the steps of: reacting a bromine compound represented by the formula 2 and 2,3-butanedione monoxime represented by the formula 3 in the presence of a base to produce an oxime-based ketone compound; reducing the oxime-based ketone compound or condensing the oxime-based ketone compound with a hydroxy amine to produce an oxime-based alc. compound or a dioxime-based compound; reacting the oxime-based alc. compound or the dioxime-based compound with a Pr fluoride compound in the presence of a base. In the formula, R1 is trifluoromethyl, R2 is a Ph group, X is CH or N, and Y is O or NH.

L85 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2004:370917 CAPLUS Full-text

DOCUMENT NUMBER: 140:391189

TITLE: Preparation of furan derivatives for treatment of

osteoporosis

INVENTOR(S): Kim, Jung-Keun; Kim, Se-Won; Oh, Kwi-Ok; Ko, Seon Yle;

Kim, Jong Yeo; Lee, Byung-Eui; Kim, Bum Tae; Lee,

Yeon Soo; Min, Yong Ki; Park, No Kyun

PATENT ASSIGNEE(S): Oscotec Inc., S. Korea; Korea Research Institute of

Chemical Technology

SOURCE: PCT Int. Appl., 76 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PAT	PATENT NO.					KIND DATE			APPLICATION NO.							DATE		
WO	2004	0378	04		A1 20040506			WO 2003-KR2231							20031022			
	W:	ΑE,	AG,	AL,	ΑM,	ΑT,	ΑU,	ΑZ,	BA,	BE	3,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	ΕC	Ξ,	EE,	EG,	ES,	FI,	GB,	GD,	GE,
		GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JE	₽,	KE,	KG,	KP,	KΖ,	LC,	LK,	LR,
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN	٧,	MW,	MX,	MZ,	NΙ,	NO,	NΖ,	OM,
		PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE	Ξ,	SG,	SK,	SL,	SY,	ΤJ,	TM,	TN,
		TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN	V,	YU,	ZA,	ZM,	ZW			
	RW: GH, GM, KE, LS		LS,	MW,	MZ,	SD,	SL,	SZ	Ζ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,	BY,		
		KG,	KΖ,	MD,	RU,	ТJ,	TM,	ΑT,	BE,	BO	3,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,
		FI,	FR,	GB,	GR,	HU,	ΙE,	ΙΤ,	LU,	MC	Ξ,	NL,	PT,	RO,	SE,	SI,	SK,	TR,
		BF,	ΒJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GÇ	2,	GW,	$\mathrm{ML}_{\prime}$	MR,	ΝE,	SN,	TD,	ΤG
KR	2004	0355	59		Α		2004	KR 2003-72536					20031017			017		
AU	2003	2730	96		A1		2004	0513		AU 2003-273096		96		200310		022		
JP	2006	5152	76		Τ		2006	0525		JΡ	20	004-	5465.	35		2	0031	022
US	2006	0004	880		A1		2006	0105		US	20	05-	5317	14		2	0050	418
KR	2005	0804	52		Α		2005	0812		KR	20	05-	5645	4		2	0050	628
PRIORIT?	Y APP	LN.	INFO	.:						KR	20	02-	6467	0		A 2	0021	022
										KR	20	03-	7253	6		A 2	0031	017
										WO	20	03-	KR22.	31		W 2	0031	022

OTHER SOURCE(S): MARPAT 140:391189

GΙ

AB The title compds. I [wherein X = H, (un)substituted OH, or NH2; Y = SC(=NH)NH2, (un)substituted OH, or NH2] or pharmaceutically acceptable salts thereof are prepd for the treatment of bone disease. For example, the compound II was obtained by extraction from a plant rehmannia glutinosa libosch. I showed strong effect on bone proliferation with the side effect reduced. I also showed high inhibition rate against osteoclast formation at different concns. Formulations containing I as an active ingredient were also described.

L85 ANSWER 12 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2003:319855 CAPLUS Full-text

DOCUMENT NUMBER: 138:321015

TITLE: Process for the monoesterification of dihydroxybenzene

using carboxylic anhydrides or halides

INVENTOR(S): Lee, Yeon-Soo; Kim, Bum-Tae; Min, Yong-Ki;

Park, No-Kyun; Kim, Ki-Ho; Kim, Ki-Soo; Park, No-Kyun

PATENT ASSIGNEE(S): Bioland Co., Ltd., S. Korea; Korea Research Institute

of Chemical Technology

SOURCE: PCT Int. Appl., 12 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

P	PATENT NO.					KIND DATE			APPLICATION NO.						DATE				
M	WO 2003033449				A1	A1 20030424			WO 2002-KR1915						20021014				
		W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,	
			CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	
			GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KP,	KΖ,	LC,	LK,	LR,	LS,	
			LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,	PL,	
			PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ΤJ,	TM,	TN,	TR,	TT,	TZ,	UA,	
			UG,	US,	UZ,	VN,	YU,	ZA,	ZM,	ZW									
		RW:	GH,	GM,	ΚE,	LS,	MW,	ΜZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,	BY,	
			KG,	KΖ,	MD,	RU,	ТJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	
			FI,	FR,	GB,	GR,	ΙE,	ΙΤ,	LU,	MC,	NL,	PT,	SE,	SK,	TR,	BF,	ВJ,	CF,	
			CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	ΤG				
K	KR 2003032301					Α	20030426				KR 2001-64008						20011017		
A	AU 2002353549					A1		2003	0428	AU 2002-353549						20021014			
U	US 20040260114					A1		20041223 US 2004-490673							20040324				
U	US 6933403 B2						20050823												
PRIORI	RIORITY APPLN. INFO.:										KR 2001-64008					A 2	0011	017	
										,	WO 2	002-	KR19:	15		W 2	0021	014	
OTHER	SO	URCE	(S):			CASI	REAC	T 13	8:32	1015	; MA	RPAT	138	:321	015				
AB 1	Dih	nydro	xybe	enzer	nes (	e.g.	, hy	droc	quinc	ne)	are	mono	este	erifi	.ed	[i.e.	, th	ıe	

production of 4-(acetyloxy)phenol] by their reaction with carboxylic anhydrides (e.g., acetic anhydride) or halides in the absence of organic or inorg. bases.

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L85 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2001:924331 CAPLUS Full-text

DOCUMENT NUMBER: 136:37895

TITLE: Preparation of arbutin intermediates by stereoselective glycosylation reaction of

hydroquinones

Lee, Yeon Soo; Kim, Bum Tae; Min, Yong Ki; INVENTOR(S):

Park, No Kyum; Kim, Ki Ho; Lee, Jae Seob; Jeoung,

See Wha; Kim, Ki Soo

PATENT ASSIGNEE(S): Bioland Co., Ltd., S. Korea; Korea Research Institute

of Chemical Technology

SOURCE: U.S. Pat. Appl. Publ., 4 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 20010053846	A1	20011220	US 2001-838841		20010420
US 6388103	B2	20020514			
PRIORITY APPLN. INFO.:			KR 2000-27129	Α	20000519
OTHER SOURCE(S):	CASREA	ACT 136:37895	; MARPAT 136:37895		
GT					

AB The invention is related to a preparation method of arbutin intermediates I wherein R is hydrogen, alkyl or cycloalkyl group with 1 to 10 carbon, or aliphatic or aromatic acyl group with 1 to 10 carbon by stereoselective glycosylation reaction of hydroquinones with penta-acetyl- $\beta$ -D-glucose in the presence of Lewis-acid and base catalysts. Thus, stereoselective glycosylation of mono-benzoyl hydroquinone with penta-acetyl- $\beta$ -D- glucose in the presence of NEt3 and borontrifluoride diethyl-etherate as Lewis-acid catalyst in CH2Cl2 gave benzoyl tetra-acetylarbutin in 90 % yield.

=> file medline embase biosis wpix FILE 'MEDLINE' ENTERED AT 14:25:22 ON 16 APR 2008

FILE 'EMBASE' ENTERED AT 14:25:22 ON 16 APR 2008 Copyright (c) 2008 Elsevier B.V. All rights reserved.

FILE 'BIOSIS' ENTERED AT 14:25:22 ON 16 APR 2008 Copyright (c) 2008 The Thomson Corporation

FILE 'WPIX' ENTERED AT 14:25:22 ON 16 APR 2008 COPYRIGHT (C) 2008 THE THOMSON CORPORATION

=> s L85 L87 14 L85

=> dup rem L85 L87

FILE 'CAPLUS' ENTERED AT 14:25:36 ON 16 APR 2008

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'WPIX' ENTERED AT 14:25:36 ON 16 APR 2008

COPYRIGHT (C) 2008 THE THOMSON CORPORATION

PROCESSING COMPLETED FOR L85

PROCESSING COMPLETED FOR L87

L88

15 DUP REM L85 L87 (12 DUPLICATES REMOVED)

ANSWERS '1-13' FROM FILE CAPLUS

ANSWERS '14-15' FROM FILE WPIX

=> d iall L88 14-15

L88 ANSWER 14 OF 15 WPIX COPYRIGHT 2008 THE THOMSON CORP on STN

ACCESSION NUMBER: 2007-338836 [32] WPIX Full-text
DOC. NO. CPI: C2007-123728 [32]
TITLE: Method for preparing alkyl lactate with high yield and

high purity from lactide through alcoholysis using lipase

DERWENT CLASS:

D16; E17

INVENTOR:

HEO J N; KIM B T; LEE W G; LEE Y S; MIN Y K; PARK N K

PATENT ASSIGNEE:

(KORE-N) KOREA RES INST CHEM TECHNOLOGY

COUNTRY COUNT: - 7

PATENT INFORMATION:

PATENT NO KIND DATE WEEK LA PG MAIN IPC \_\_\_\_\_

KR 592794 B1 20060628 (200732)\* KO [1]

APPLICATION DETAILS:

APPLICATION DATE PATENT NO KIND

-----

KR 592794 B1 KR 2005-8936 20050201

PRIORITY APPLN. INFO: KR 2005-1043 20050106

INT. PATENT CLASSIF.:

IPC ORIGINAL: C12P0041-00 [I,A]; C12P0041-00 [I,C]; C12P0007-40 [I,C];

C12P0007-56 [I,A]

BASIC ABSTRACT:

KR 592794 B1 UPAB: 20070521

NOVELTY - A method for preparing alkyl lactate is provided to obtain alkyl SS-(L)-O-lactyl lactate and/or alkyl R-(D)-lactate with high yield and high optical purity from racemic lactide or R- or S-isomer thereof.

DETAILED DESCRIPTION - Preparation of alkyl SS-(L)-O-lactyl lactate of formula (2b) and alkyl R-(D)-lactate of formula (3a) comprises alcoholizing a racemic lactide of formula(1) at a temperature of 0-80degreesC for 1-500 hours in the presence of a lipase enzyme catalyst derived from Candida antarctica.

R=1-10C saturated or unsaturated alkyl. MANUAL CODE:

D05-A02C; D05-C; E10-E04D2; E11-G03; E11-M

L88 ANSWER 15 OF 15 WPIX COPYRIGHT 2008 THE THOMSON CORP on STN

ACCESSION NUMBER: 2004-632320 [61] WPIX Full-text CROSS REFERENCE: 2003-826059

C2004-227157 [61] DOC. NO. CPI:

TITLE: Fluorine-substituted heterocyclic compounds as intermediate for synthesis of agrochemicals and

medicaments and method for preparing the same

DERWENT CLASS:

B03; C02; E13 KIM B T; LEE Y S; MIN Y G; PARK N G INVENTOR: PATENT ASSIGNEE: (KORE-N) KOREA RES INST CHEM TECHNOLOGY

COUNTRY COUNT:

PATENT INFORMATION:

PATENT NO KIND DATE WEEK LA PG MAIN IPC

KR 2004043142 A 20040522 (200461)\* KO 1[10]

APPLICATION DETAILS:

PATENT NO KIND APPLICATION DATE

\_\_\_\_\_\_

KR 2004043142 A

KR 2004-21097 20040329

PRIORITY APPLN. INFO: KR 2004-21097 20040329

INT. PATENT CLASSIF.:

MAIN: C07D239-36

BASIC ABSTRACT:

KR 2004043142 A UPAB: 20060122

NOVELTY - A fluorine-substituted heterocyclic compound as an intermediate for synthesis of agrochemicals and medicaments and a method for preparing the same are provided, thereby regio-selectively preparing the 5-fluoro-pyrazole derivative and 4-fluoro-6-hydroxy pyrimidine derivative in higher yield.

DETAILED DESCRIPTION - A method for preparing a 4-fluoro-6-hydroxy pyrimidine derivative with substituted phenyl at C3 or C4 position represented by the formula(2) comprises reacting a methyl 2-fluoroalkyl 2-phenylacetate derivative of the formula(3) with a substituted guanidine derivative(R2C(NH2)=NH) in the presence of an solvent, wherein X is hydrogen, halogen, C1-4 alkyl, C1-4 alkoxy or C1-4 arylalkyloxy; RF is fluorine or trifluoromethyl; R3 is hydrogen, C1-4 alkyl, C1-4 aryl or C1-4 arylalkyl; the solvent is acetonitrile, 1,4-dioxane, or 5 to 30 % 1,4-dioxane solution; and the reaction temperature is 60 to 120 deg. C. MANUAL CODE: CPI: B07-D08; B07-D12; B10-H02A; B11-C01; C07-D08;

C07-D12; C10-H02A; C11-C01; C14-T; E07-D08; E07-D12

=> file registry
FILE 'REGISTRY' ENTERED AT 14:25:56 ON 16 APR 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 15 APR 2008 HIGHEST RN 1015083-77-8 DICTIONARY FILE UPDATES: 15 APR 2008 HIGHEST RN 1015083-77-8

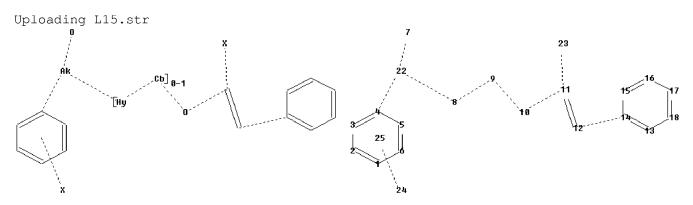
New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

# http://www.cas.org/support/stngen/stndoc/properties.html



chain nodes :
7 8 9 10 11 12 22 23 24
ring nodes :
1 2 3 4 5 6 13 14 15 16 17 18
chain bonds :
4-22 7-22 8-9 8-22 9-10 10-11 11-12 11-23 12-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18
exact/norm bonds :
4-22 7-22 8-9 8-22 9-10 10-11 11-23 12-14
exact bonds :
11-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18

# Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:CLASS

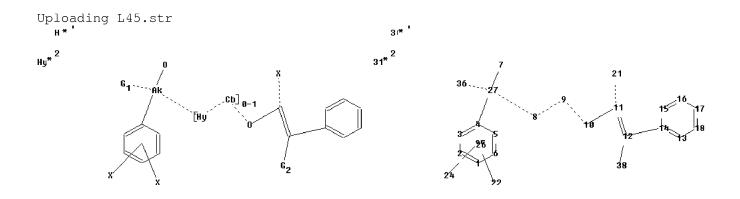
11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 22:CLASS 23:CLASS 24:CLASS

25:CLASS

Generic attributes :

Saturation : Unsaturated

Element Count : Node 8: Limited N,N1



chain nodes : 7 8 9 10 11 12 21 22 24 27 30 31 36 38 ring nodes : 1 2 3 4 5 6 13 14 15 16 17 18 chain bonds : 4-27 7-27 8-9 8-27 9-10 10-11 11-12 11-21 12-14 12-38 27-36 ring bonds :  $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 13-14 \quad 13-18 \quad 14-15 \quad 15-16 \quad 16-17 \quad 17-18$ exact/norm bonds : 4-27 8-9 8-27 9-10 11-21 12-38 27-36 exact bonds : 7-27 10-11 11-12 12-14 normalized bonds : 1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18

G1:[\*1],[\*2]

G2:H,CF3

Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 21:CLASS 22:CLASS 24:CLASS 25:CLASS 26:CLASS 27:Atom 30:CLASS 31:Atom 36:CLASS 38:CLASS

Generic attributes :

9:

Saturation : Unsaturated

27:

Saturation : Saturated

31:

Saturation : Unsaturated

Element Count : Node 8: Limited

N, N2 C, C3

Node 9: Limited

C, C6

Node 31: Limited

N,N3 C,C3

Uploading L59.str

Hy\*

28\*

28\*

28\*

28\*

19

19

10

11

15

16

16

7 8 9 10 19 20 21 24 27 28 33 35

ring nodes :

chain nodes :

1 2 3 4 5 6 11 12 13 14 15 16

chain bonds :

4-24 7-24 8-9 8-24 9-10 10-35 12-35 19-35 24-33

ring bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 11-12 \quad 11-16 \quad 12-13 \quad 13-14 \quad 14-15 \quad 15-16$ 

exact/norm bonds :

4-24 8-9 8-24 9-10 10-35 12-35 19-35 24-33

exact bonds :

7 - 24

normalized bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 11-12 \quad 11-16 \quad 12-13 \quad 13-14 \quad 14-15 \quad 15-16$ 

G1:[\*1],[\*2]

G2:H,CF3

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 19:Atom 20:Atom 21:Atom

22:CLASS 23:CLASS

24:Atom 27:CLASS 28:Atom 33:CLASS 35:CLASS

Generic attributes :

9:

Saturation : Unsaturated

24:

Saturation : Saturated

28:

Saturation : Unsaturated

35:

Saturation : Unsaturated

Element Count : Node 8: Limited

N, N2 C, C3

Node 9: Limited

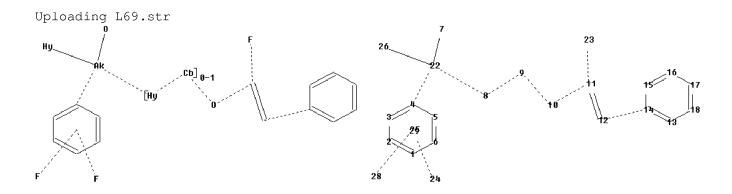
C,C6

Node 28: Limited

N,N3 C,C3

Node 35: Limited

C,C2-4



chain nodes :

7 8 9 10 11 12 22 23 24 26 28

ring nodes :

1 2 3 4 5 6 13 14 15 16 17 18

chain bonds :

 $4-22 \quad 7-22 \quad 8-9 \quad 8-22 \quad 9-10 \quad 10-11 \quad 11-12 \quad 11-23 \quad 12-14 \quad 22-26$ 

ring bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 4-5 \quad 5-6 \quad 13-14 \quad 13-18 \quad 14-15 \quad 15-16 \quad 16-17 \quad 17-18$ 

exact/norm bonds :

4-22 8-9 8-22 9-10 10-11 11-23 12-14 22-26

exact bonds :

7-22 11-12

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 22:CLASS 23:CLASS

25:CLASS 26:Atom 28:CLASS 29:CLASS

Generic attributes :

9:

Saturation : Unsaturated

Element Count : Node 8: Limited N,N1

Node 26: Limited

N, N3 C, C3

=> file caplus
FILE 'CAPLUS' ENTERED AT 14:25:59 ON 16 APR 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

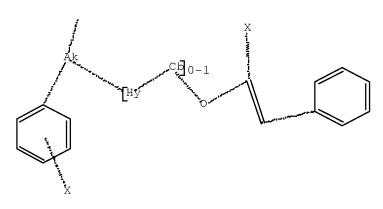
Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 16 Apr 2008 VOL 148 ISS 16 FILE LAST UPDATED: 15 Apr 2008 (20080415/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html
'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

=> d stat que L18 L15 STR



Structure attributes must be viewed using STN Express query preparation.

127 SEA FILE=REGISTRY SSS FUL L15

L18 1 SEA FILE=CAPLUS ABB=ON PLU=ON L17

=> file beilstein FILE 'BEILSTEIN' ENTERED AT 14:26:07 ON 16 APR 2008 COPYRIGHT (c) 2008 Beilstein-Institut zur Foerderung der Chemischen Wissenschaften licensed to Beilstein GmbH and MDL Information Systems GmbH

FILE LAST UPDATED ON April 1, 2008

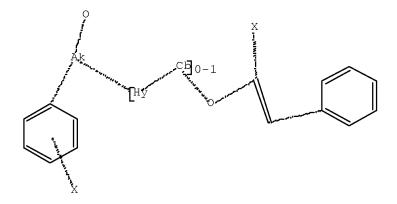
FILE COVERS 1771 TO 2008.
\*\*\* FILE CONTAINS 10.322,808 SUBSTANCES \*\*\*

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For mo detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

>>> Price change as of January 1st, 2008: Connect Time and Structure Search fees re-introduced. See NEWS and HELP COST <<<

=> d stat que L20 L15 STR



Structure attributes must be viewed using STN Express query preparation. L20  $\,$  0 SEA FILE=BEILSTEIN SSS FUL L15

100.0% PROCESSED 109 ITERATIONS 0 ANSWERS SEARCH TIME: 00.00.01

=> file marpat

FILE 'MARPAT' ENTERED AT 14:26:24 ON 16 APR 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 American Chemical Society (ACS)

FILE CONTENT: 1961-PRESENT VOL 148 ISS 14 (20080411/ED)

SOME MARPAT RECORDS ARE DERIVED FROM INPI DATA FOR 1961-1987

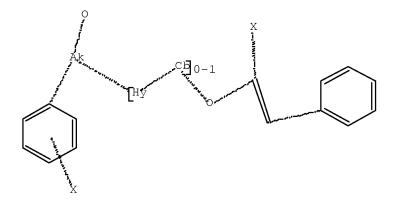
MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES (COVERAGE TO THESE DATES IS NOT COMPLETE):

US 20080051413 28 FEB 2008 DE 102006039038 21 FEB 2008 EΡ 1889831 20 FEB 2008 JΡ 2008044933 28 FEB 2008 WO 2008028336 13 MAR 2008 GB 2440819 13 FEB 2008 2904973 22 FEB 2008 FR RU 2317993 27 FEB 2008 2593150 06 JAN 2008 CA

Expanded G-group definition display now available.

Effective December 15th the iteration and answer limits in MARPAT have increased from 100,000 to 200,000 for both on-line and batch searches. For more information on MARPAT search limits, type HELP SLIMITS at an arrow prompt.

=> d stat que L62 L15 STR



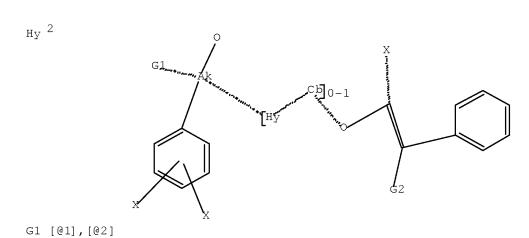
Structure attributes must be viewed using STN Express query preparation.

L22 215 SEA FILE=MARPAT SSS FUL L15

L45 STR

<sub>H</sub> 1

G2 H,CF3



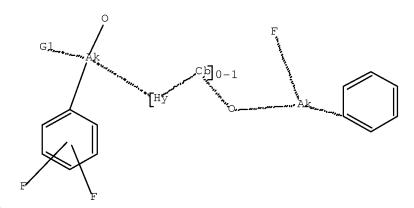
Structure attributes must be viewed using STN Express query preparation.

L47 99 SEA FILE=MARPAT SUB=L22 SSS FUL L45

L59 STR

H 1

Hy 2

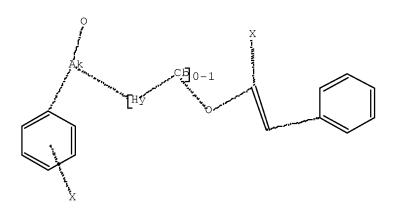


G1 [@1],[@2] G2 H,CF3

Structure attributes must be viewed using STN Express query preparation.

L61 23 SEA FILE=MARPAT SUB=L47 SSS FUL L59 L62 22 SEA FILE=MARPAT ABB=ON PLU=ON L61/COM

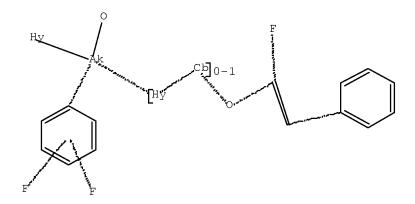
=> d stat que L72 L15 STR



Structure attributes must be viewed using STN Express query preparation.

L22 215 SEA FILE=MARPAT SSS FUL L15

L69 STR



Structure attributes must be viewed using STN Express query preparation.

L71 17 SEA FILE=MARPAT SUB=L22 SSS FUL L69
L72 17 SEA FILE=MARPAT ABB=ON PLU=ON L71/COM

=> s L62 or L72

L89 36 L62 OR L72

=> d ibib abs hitstr L18 tot; d ibib abs qhit L89 1-36
YOU HAVE REQUESTED DATA FROM FILE 'CAPLUS' - CONTINUE? (Y)/N:y

L18 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2005:141060 CAPLUS <u>Full-text</u>

DOCUMENT NUMBER: 142:240437

TITLE: Preparation of triazolylmethanol derivatives as

antifungal agents

INVENTOR(S): Kim, Bum Tae; Min, Yong Ki; Lee, Yeon Soo; Park, No

Kyun; Kim, Woo Jung

PATENT ASSIGNEE(S): Korea Research Institute of Chemical Technology, S.

Korea

SOURCE: PCT Int. Appl., 58 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT NO.	:	KINI	) ]	DATE		APPLICATION NO.						DATE			
WO 20050145	•	A1 20050217			WO 2004-KR1996						20040809				
W: AE,	AG,	AL,	ΑM,	AT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
CN,	CO, (	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,
GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KP,	KΖ,	LC,	LK,
LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,	NO,
NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	ΤJ,
TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW	
RW: BW,	GH,	GM,	KΕ,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,
AZ,	BY,	KG,	KΖ,	MD,	RU,	ΤJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	ΙΤ,	LU,	MC,	NL,	PL,	PT,	RO,	SE,

SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG KR 2005017962 20050223 KR 2003-55590 Α EP 1654254 20060510 EP 2004-748524 20040809 A 1 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK JP 2007502268 Τ 20070208 JP 2006-523125 20040809 US 20080027117 Α1 20080131 US 2006-566911 20060203 PRIORITY APPLN. INFO.: KR 2003-55590 A 20030812 WO 2004-KR1996 20040809 OTHER SOURCE(S): CASREACT 142:240437; MARPAT 142:240437 GΙ

Ι

$$\begin{array}{c|c}
N & \text{OH} & F \\
\hline
N & F & CF3
\end{array}$$

Title compds. represented by the formula I [wherein A = 0, 1,2,4-triazolyl-PhO-, 1,2,4-triazolone-3-yl-PhO-, imidazolone-1-yl-PhO, imidazolinone-1-yl-PhO-; R = H or CF3; R' = H or alkyl; X = H, halo, (halo)alkyl,alkoxy, 3,4-dioxyalkylene; and pharmaceutically acceptable salts, isomers or esters thereof] were prepared as antifungal agents for the treatment of humans or animals. For example, II was given in a multi-step synthesis starting from the reaction of Me (R)-lactate with morpholine. I showed antifungal activity in vivo against a wide spectrum of pathogenic fungi, such as ATCC 10231 and MYA-573, and low toxicity in oral administration.

RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of difluorophenyl triazolylmethanol derivs. as antifungal agents)

RN 844878-16-6 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol, 3-[4-[[2-(4-chlorophenyl)-1-fluoroethenyl]oxy]phenyl]- $\alpha$ -(2,4-difluorophenyl)- $\beta$ -methyl- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)-, ( $\alpha$ R, $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

```
ΙT
     844877-73-2P 844877-76-5P 844877-80-1P
     844877-81-2P 844877-82-3P 844877-83-4P
     844877-84-5P 844877-85-6P 844877-86-7P
     844877-87-8P 844877-88-9P 844877-89-0P
     844877-90-3P 844877-91-4P 844877-92-5P
     844877-93-6P 844877-94-7P 844877-95-8P
     844877-96-9P 844877-97-0P 844877-98-1P
     844877-99-2P 844878-00-8P 844878-01-9P
     844878-02-0P 844878-03-1P 844878-04-2P
     844878-05-3P 844878-06-4P 844878-07-5P
     844878-08-6P 844878-09-7P 844878-10-0P
     844878-11-1P 844878-12-2P 844878-13-3P
     844878-14-4P 844878-15-5P 844878-17-7P
     844878-18-8P 844878-19-9P 844878-20-2P
     844878-21-3P 844878-22-4P 844878-23-5P
     844878-24-6P 844878-25-7P 844878-26-8P
     844878-27-9P 844878-28-0P 844878-29-1P
     844878-30-4P 844878-31-5P 844878-32-6P
     844878-33-7P 844878-34-8P 844878-35-9P
     844878-36-0P 844878-37-1P 844878-38-2P
     844878-39-3P 844878-40-6P 844878-41-7P
     844878-42-8P 844878-43-9P 844878-44-0P
     844878-45-1P 844878-47-3P 844878-48-4P
     844878-49-5P 844878-50-8P 844878-51-9P
     844878-52-0P 844878-53-1P 844878-54-2P
     844878-55-3P 844878-56-4P 844878-57-5P
     844878-58-6P 844878-60-0P 844878-61-1P
     844878-62-2P 844878-63-3P 844878-64-4P
     844878-65-5P 844878-67-7P 844878-69-9P
     844878-71-3P 844878-73-5P 844878-75-7P
     844878-77-9P 844878-79-1P 844878-81-5P
     844878-83-7P 844878-85-9P 844878-87-1P
     844878-89-3P 844878-90-6P 844878-92-8P
     844878-94-0P 844878-96-2P 844878-98-4P
     844879-02-3P 844879-05-6P 844879-08-9P
     844879-11-4P 844879-13-6P 844879-15-8P
     844879-17-0P 844879-19-2P 844879-21-6P
     844879-23-8P 844879-25-0P 844879-26-1P
     844879-28-3P 844879-30-7P 844879-32-9P
     844879-34-1P 844879-36-3P 844879-38-5P
     844879-41-0P 844879-44-3P 844879-46-5P
     844879-48-7P 844879-50-1P 844879-53-4P
```

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of difluorophenyl triazolylmethanol derivs. as antifungal agents)

RN 844877-73-2 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -[(1R)-1-[[(1E)-2-(4-chlorophenyl)-1,3,3,3-tetrafluoro-1-propenyl]oxy]ethyl]- $\alpha$ -(2,4-difluorophenyl)-, ( $\alpha$ R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 844877-76-5 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha-[(1R)-1-[[(1Z)-2-(4-\text{chlorophenyl})-1,3,3,3-\text{tetrafluoro-1-propenyl}] \text{ oxy}] \text{ethyl}]-\alpha-(2,4-\text{difluorophenyl})-, ($\alpha R)-(9CI) (CA INDEX NAME)$ 

Absolute stereochemistry.

Double bond geometry as shown.

RN 844877-80-1 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)- $\alpha$ -[(1R)-1-[(1E)-1,3,3,3-tetrafluoro-2-[4-(trifluoromethyl)phenyl]-1-propenyl]oxy]ethyl]-, ( $\alpha$ R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

RN 844877-81-2 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)- $\alpha$ -[(1R)-1-[(1Z)-1,3,3,3-tetrafluoro-2-[4-(trifluoromethyl)phenyl]-1-propenyl]oxy]ethyl]-, ( $\alpha$ R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 844877-82-3 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)- $\alpha$ -[(1R)-1-[(1,3,3,3-tetrafluoro-2-phenyl-1-propenyl)oxy]ethyl]-, ( $\alpha$ R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

RN 844877-83-4 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)- $\alpha$ -[(1R)-1-[[2-(3,4-dimethylphenyl)-1,3,3,3-tetrafluoro-1-propenyl]oxy]ethyl]-, ( $\alpha$ R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

RN 844877-84-5 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)- $\alpha$ -[(1R)-1-[[2-(4-ethoxyphenyl)-1,3,3,3-tetrafluoro-1-propenyl]oxy]ethyl]-, ( $\alpha$ R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844877-85-6 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)- $\alpha$ -[(1R)-1-[[2-[4-(1,1-dimethylethyl)phenyl]-1,3,3,3-tetrafluoro-1-propenyl]oxy]ethyl]-, ( $\alpha$ R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

RN 844877-86-7 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -[(1R)-1-[[2-(4-bromophenyl)-1,3,3,3-tetrafluoro-1-propenyl]oxy]ethyl]- $\alpha$ -(2,4-difluorophenyl)-, ( $\alpha$ R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844877-87-8 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)- $\alpha$ -[(1R)-1-[(1E)-1,3,3,3-tetrafluoro-2-(4-methylphenyl)-1-propenyl]oxy]ethyl]-, ( $\alpha$ R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 844877-88-9 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)- $\alpha$ -[(1R)-1-[(1Z)-1,3,3,3-tetrafluoro-2-(4-methylphenyl)-1-propenyl]oxy]ethyl]-, ( $\alpha$ R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 844877-89-0 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)- $\alpha$ -[(1R)-1-[[1,3,3,3-tetrafluoro-2-(3-methoxyphenyl)-1-propenyl]oxy]ethyl]-, ( $\alpha$ R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

RN 844877-90-3 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)- $\alpha$ -[(1R)-1-[[1,3,3,3-tetrafluoro-2-[3-(trifluoromethyl)phenyl]-1-propenyl]oxy]ethyl]-, ( $\alpha$ R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

RN 844877-91-4 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)- $\alpha$ -[(1R)-1-[(1E)-1-fluoro-2-(4-phenoxyphenyl)ethenyl]oxy]ethyl]-, ( $\alpha$ R)- (CA

INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 844877-92-5 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)- $\alpha$ -[(1R)-1-[[1-fluoro-2-(4-methoxyphenyl)ethenyl]oxy]ethyl]-, ( $\alpha$ R)- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844877-93-6 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)- $\alpha$ -[(1R)-1-[[2-(3,5-dimethylphenyl)-1-fluoroethenyl]oxy]ethyl]-, ( $\alpha$ R)- (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

RN 844877-94-7 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)- $\alpha$ -[(1R)-1-[[2-(4-ethylphenyl)-1-fluoroethenyl]oxy]ethyl]-, ( $\alpha$ R)- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844877-95-8 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -[(1R)-1-[[2-(4-butylphenyl)-1-fluoroethenyl]oxy]ethyl]- $\alpha$ -(2,4-difluorophenyl)-, ( $\alpha$ R)- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844877-96-9 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)- $\alpha$ -[(1R)-1-[[1-fluoro-2-(4-methylphenyl)ethenyl]oxy]ethyl]-, ( $\alpha$ R)- (CA INDEX NAME)

RN 844877-97-0 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)- $\alpha$ -[(1R)-1-[[1-fluoro-2-(4-fluorophenyl)ethenyl]oxy]ethyl]-, ( $\alpha$ R)- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844877-98-1 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -[(1R)-1-[[2-(1,3-benzodioxol-5-yl)-1-fluoroethenyl]oxy]ethyl]- $\alpha$ -(2,4-difluorophenyl)-, ( $\alpha$ R)- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844877-99-2 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)- $\alpha$ -[(1R)-1-[[(1Z)-1-fluoro-2-(4-phenoxyphenyl)ethenyl]oxy]ethyl]-, ( $\alpha$ R)- (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 844878-00-8 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)- $\alpha$ -[(1R)-1-[[2-[4-(1,1-dimethylethyl)phenyl]-1-fluoroethenyl]oxy]ethyl]-, ( $\alpha$ R)-(CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844878-01-9 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)- $\beta$ -methyl-3- [4-[[1,3,3,3-tetrafluoro-2-(4-methylphenyl)-1-propenyl]oxy]phenyl]- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)-, ( $\alpha$ R, $\beta$ R)- (9CI) (CA INDEX NAME)

RN 844878-02-0 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol, 3-[4-[[2-(4-chlorophenyl)-1,3,3,3-tetrafluoro-1-propenyl]oxy]phenyl]- $\alpha$ -(2,4-difluorophenyl)- $\beta$ -methyl- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)-, ( $\alpha$ R, $\beta$ R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

RN 844878-03-1 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)- $\beta$ -methyl-3- [4-[[1,3,3,3-tetrafluoro-2-(4-fluorophenyl)-1-propenyl]oxy]phenyl]- $\alpha$ - (1H-1,2,4-triazol-1-ylmethyl)-, ( $\alpha$ R, $\beta$ R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844878-04-2 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol, 3-[4-[[2-(1,3-benzodioxol-5-yl)-1,3,3,3-tetrafluoro-1-propenyl]oxy]phenyl]- $\alpha$ -(2,4-difluorophenyl)- $\beta$ -methyl- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)-, ( $\alpha$ R, $\beta$ R)- (9CI) (CA INDEX NAME)

RN 844878-05-3 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)- $\beta$ -methyl-3-[4-[[1,3,3,3-tetrafluoro-2-[3-(trifluoromethyl)phenyl]-1-propenyl]oxy]phenyl]- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)-, ( $\alpha$ R,  $\beta$ R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

RN 844878-06-4 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)- $\beta$ -methyl-3- [4-[[1,3,3,3-tetrafluoro-2-(3-fluorophenyl)-1-propenyl]oxy]phenyl]- $\alpha$ - (1H-1,2,4-triazol-1-ylmethyl)-, ( $\alpha$ R, $\beta$ R)- (9CI) (CA INDEX NAME)

RN 844878-07-5 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol, 3-[4-[[2-(3,5-dichlorophenyl)-1,3,3,3-tetrafluoro-1-propenyl]oxy]phenyl]- $\alpha$ -(2,4-difluorophenyl)- $\beta$ -methyl- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)-, ( $\alpha$ R, $\beta$ R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844878-08-6 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)- $\beta$ -methyl-3-[4-[[1,3,3,3-tetrafluoro-2-(4-methoxyphenyl)-1-propenyl]oxy]phenyl]- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)-, ( $\alpha$ R, $\beta$ R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844878-09-7 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)- $\beta$ -methyl-3-[4-[[1,3,3,3-tetrafluoro-2-(3-methoxyphenyl)-1-propenyl]oxy]phenyl]- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)-, ( $\alpha$ R, $\beta$ R)- (9CI) (CA INDEX NAME)

RN 844878-10-0 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)-3-[4-[[2-(3,4-dimethylphenyl)-1,3,3,3-tetrafluoro-1-propenyl]oxy]phenyl]- $\beta$ -methyl- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)-, ( $\alpha$ R, $\beta$ R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

RN 844878-11-1 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)-3-[4-[[2-(3,5-dimethylphenyl)-1,3,3,3-tetrafluoro-1-propenyl]oxy]phenyl]- $\beta$ -methyl- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)-, ( $\alpha$ R, $\beta$ R)- (9CI) (CA INDEX NAME)

RN 844878-12-2 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)-3-[4-[[2-[4-(1,1-dimethylethyl)phenyl]-1,3,3,3-tetrafluoro-1-propenyl]oxy]phenyl]- $\beta$ -methyl- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)-, ( $\alpha$ R, $\beta$ R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844878-13-3 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)-3-[4-[[1-fluoro-2-(4-phenoxyphenyl)ethenyl]oxy]phenyl]- $\beta$ -methyl- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)-, ( $\alpha$ R, $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

RN 844878-14-4 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)-3-[4-[[1-fluoro-2-(3-methylphenyl)ethenyl]oxy]phenyl]- $\beta$ -methyl- $\alpha$ -(1H-1,2,4-triazol-1-vlmethyl)-, ( $\alpha$ R, $\beta$ R)- (CA INDEX NAME)

RN 844878-15-5 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)-3-[4-[[2-(4-ethoxyphenyl)-1,3,3,3-tetrafluoro-1-propenyl]oxy]phenyl]- $\beta$ -methyl- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)-, ( $\alpha$ R, $\beta$ R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844878-17-7 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)-3-[4-[[1-fluoro-2-(4-fluorophenyl)ethenyl]oxy]phenyl]- $\beta$ -methyl- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)-, ( $\alpha$ R, $\beta$ R)- (CA INDEX NAME)

RN 844878-18-8 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)-3-[4-[[1-fluoro-2-[4-(trifluoromethyl)phenyl]ethenyl]oxy]phenyl]- $\beta$ -methyl- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)-, ( $\alpha$ R,  $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844878-19-9 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)-3-[4-[(1-fluoro-2-phenylethenyl)oxy]phenyl]- $\beta$ -methyl- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)-, ( $\alpha$ R, $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844878-20-2 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol, 3-[4-[[2-(3-chlorophenyl)-1-fluoroethenyl]oxy]phenyl]- $\alpha$ -(2,4-difluorophenyl)- $\beta$ -methyl- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)-, ( $\alpha$ R, $\beta$ R)- (CA INDEX NAME)

RN 844878-21-3 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)-3-[4-[[1-fluoro-2-[3-(1-methylethoxy)phenyl]ethenyl]oxy]phenyl]- $\beta$ -methyl- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)-, ( $\alpha$ R, $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

RN 844878-22-4 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)-3-[4-[[1-fluoro-2-(3-methoxyphenyl)ethenyl]oxy]phenyl]- $\beta$ -methyl- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)-, ( $\alpha$ R, $\beta$ R)- (CA INDEX NAME)

RN 844878-23-5 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)-3-[4-[[2-(4-ethylphenyl)-1-fluoroethenyl]oxy]phenyl]- $\beta$ -methyl- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)-, ( $\alpha$ R, $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844878-24-6 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)-3-[4-[[2-(3,5-dimethylphenyl)-1-fluoroethenyl]oxy]phenyl]- $\beta$ -methyl- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)-, ( $\alpha$ R, $\beta$ R)- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844878-25-7 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)- $\beta$ -methyl-3- [4-[[1,3,3,3-tetrafluoro-2-(3-methylphenyl)-1-propenyl]oxy]phenyl]- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)-, ( $\alpha$ R, $\beta$ R)- (9CI) (CA INDEX NAME)

RN 844878-26-8 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol, 3-[4-[[2-(4-butylphenyl)-1,3,3,3-tetrafluoro-1-propenyl]oxy]phenyl]- $\alpha$ -(2,4-difluorophenyl)- $\beta$ -methyl- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)-, ( $\alpha$ R, $\beta$ R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

RN 844878-27-9 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)- $\beta$ -methyl-3-[4-[[1,3,3,3-tetrafluoro-2-(4-phenoxyphenyl)-1-propenyl]oxy]phenyl]-  $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)-, ( $\alpha$ R, $\beta$ R)- (9CI) (CA INDEX NAME)

RN 844878-28-0 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)-3-[4-[[1-fluoro-2-(3-methylphenyl)ethenyl]oxy]phenyl]- $\beta$ -methyl- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)- (CA INDEX NAME)

RN 844878-29-1 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol, 3-[4-[[2-(3-chlorophenyl)-1-fluoroethenyl]oxy]phenyl]- $\alpha$ -(2,4-difluorophenyl)- $\beta$ -methyl- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)- (CA INDEX NAME)

RN 844878-30-4 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)-3-[4-[(1-fluoro-2-phenylethenyl)oxy]phenyl]- $\beta$ -methyl- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)- (CA INDEX NAME)

RN 844878-31-5 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)- $\beta$ -methyl-3- [4-[(1,3,3,3-tetrafluoro-2-phenyl-1-propenyl)oxy]phenyl]- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)- (9CI) (CA INDEX NAME)

RN 844878-32-6 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)-3-[4-[[1-fluoro-2-(4-fluorophenyl)ethenyl]oxy]phenyl]- $\beta$ -methyl- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)- (CA INDEX NAME)

$$\begin{array}{c|c}
 & F \\
 & Me \\
 & N \\
 & CH_2 - CH \\
 & CH \\
 & N \\
 &$$

RN 844878-33-7 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol, 3-[4-[[2-(1,3-benzodioxol-5-yl)-1,3,3,3-tetrafluoro-1-propenyl]oxy]phenyl]- $\alpha$ -(2,4-difluorophenyl)- $\beta$ -methyl- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)- (9CI) (CA INDEX NAME)

RN 844878-34-8 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)- $\beta$ -methyl-3- [4-[[1,3,3,3-tetrafluoro-2-(3-methoxyphenyl)-1-propenyl]oxy]phenyl]-  $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & F \\
 & Me \\
 & N \\
 & CH_2 - CH$$

RN 844878-35-9 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $3-[4-[[2-(3,5-dichlorophenyl)-1,3,3,3-tetrafluoro-1-propenyl]oxy]phenyl]-<math>\alpha$ -(2,4-difluorophenyl)- $\beta$ -methyl- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)- (9CI) (CA INDEX NAME)

RN 844878-36-0 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)-3-[4-[[1-fluoro-2-(4-methylphenyl)ethenyl]oxy]phenyl]- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)- (CA INDEX NAME)

RN 844878-37-1 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)-3-[4-[[1-fluoro-2-(4-methoxyphenyl)ethenyl]oxy]phenyl]- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)- (CA INDEX NAME)

RN 844878-38-2 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)-3-[4-[(1-fluoro-2-phenylethenyl)oxy]phenyl]- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)- (CA INDEX NAME)

RN 844878-39-3 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol, 3-[4-[[2-(4-chlorophenyl)-1-fluoroethenyl]oxy]phenyl]- $\alpha$ -(2,4-difluorophenyl)- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)- (CA INDEX NAME)

$$\begin{array}{c} & & & & & \\ & & & & \\ & & & & \\ N & & & \\ N & & & \\ \end{array}$$

RN 844878-40-6 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)-3-[4-[[1-fluoro-2-(3-methylphenyl)ethenyl]oxy]phenyl]- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)- (CA INDEX NAME)

RN 844878-41-7 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)-3-[4-[(1,3,3,3-tetrafluoro-2-phenyl-1-propenyl)oxy]phenyl]- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)- (9CI) (CA INDEX NAME)

RN 844878-42-8 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)-3-[4-[[1,3,3,3-tetrafluoro-2-(4-methylphenyl)-1-propenyl]oxy]phenyl]- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)- (9CI) (CA INDEX NAME)

RN 844878-43-9 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol, 3-[4-[[2-(4-chlorophenyl)-1,3,3,3-tetrafluoro-1-propenyl]oxy]phenyl]- $\alpha$ -(2,4-difluorophenyl)- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)- (9CI) (CA INDEX NAME)

RN 844878-44-0 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)-3-[4-[[1,3,3,3-tetrafluoro-2-[3-(trifluoromethyl)phenyl]-1-propenyl]oxy]phenyl]- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)- (9CI) (CA INDEX NAME)

RN 844878-45-1 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol, 3-[4-[[2-(1,3-benzodioxol-5-yl)-1,3,3,3-tetrafluoro-1-propenyl]oxy]phenyl]- $\alpha$ -(2,4-difluorophenyl)- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)- (9CI) (CA INDEX NAME)

RN 844878-47-3 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)-3-[4-[[1,3,3,3-tetrafluoro-2-(3-methylphenyl)-1-propenyl]oxy]phenyl]- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)- (9CI) (CA INDEX NAME)

RN 844878-48-4 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol, 3-[4-[[2-(3-chlorophenyl)-1,3,3,3-tetrafluoro-1-propenyl]oxy]phenyl]- $\alpha$ -(2,4-difluorophenyl)- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & F \\
 & N \\
 & N \\
 & CH_2 - C \\
 & CH_2 - N \\
 & N \\
 & N
\end{array}$$

$$\begin{array}{c|c}
 & CF_3 \\
 & C \\$$

RN 844878-49-5 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)-3-[4-[[1,3,3,3-tetrafluoro-2-(3-fluorophenyl)-1-propenyl]oxy]phenyl]- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & F \\
 & N \\
 & CH_2 - C - CH_2 - N \\
 & N \\
 &$$

RN 844878-50-8 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)-3-[4-[[1,3,3,3-tetrafluoro-2-(3-methoxyphenyl)-1-propenyl]oxy]phenyl]- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)- (9CI) (CA INDEX NAME)

RN 844878-51-9 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)-3-[4-[[2-(3,5-dimethylphenyl)-1-fluoroethenyl]oxy]phenyl]- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)- (CA INDEX NAME)

RN 844878-52-0 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)-3-[4-[[1-fluoro-2-[3-(1-methylethoxy)phenyl]ethenyl]oxy]phenyl]- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)- (CA INDEX NAME)

RN 844878-53-1 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)-3-[4-[[1-fluoro-2-(4-fluorophenyl)ethenyl]oxy]phenyl]- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)- (CA INDEX NAME)

RN 844878-54-2 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol, 3-[4-[[2-(3-chlorophenyl)-1-fluoroethenyl]oxy]phenyl]- $\alpha$ -(2,4-difluorophenyl)- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)- (CA INDEX NAME)

RN 844878-55-3 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol, 3-[4-[[2-(4-chloro-3-methylphenyl)-1-fluoroethenyl]oxy]phenyl]- $\alpha$ -(2,4-difluorophenyl)- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)- (CA INDEX NAME)

RN 844878-56-4 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol, 3-[4-[[2-(1,3-benzodioxol-5-yl)-1-fluoroethenyl]oxy]phenyl]- $\alpha$ -(2,4-difluorophenyl)- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)- (CA INDEX NAME)

RN 844878-57-5 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $\alpha$ -(2,4-difluorophenyl)-3-[4-[[2-(3,5-dimethylphenyl)-1,3,3,3-tetrafluoro-1-propenyl]oxy]phenyl]- $\alpha$ -(1H-1,2,4-triazol-1-ylmethyl)- (9CI) (CA INDEX NAME)

RN 844878-58-6 CAPLUS

CN 1H-1,2,4-Triazole-1-ethanol,  $3-[4-[[2-(4-butylphenyl)-1-fluoroethenyl]oxy]phenyl]-\alpha-(2,4-difluorophenyl)-\alpha-(1H-1,2,4-triazol-1-ylmethyl)- (CA INDEX NAME)$ 

RN 844878-60-0 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 2-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-4-[4-[[1-fluoro-2-(3-methylphenyl)ethenyl]oxy]phenyl]-2,4-dihydro- (CA INDEX NAME)

RN 844878-61-1 CAPLUS

CN 2H-Imidazol-2-one, 1-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-3-[4-[[1-fluoro-2-(4-methoxyphenyl)ethenyl]oxy]phenyl]-1,3-dihydro- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

RN 844878-62-2 CAPLUS

CN 2-Imidazolidinone, 1-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-3-[4-[[1-fluoro-2-(4-methoxyphenyl)ethenyl]oxy]phenyl]- (CA INDEX NAME)

RN 844878-63-3 CAPLUS

CN 2H-Imidazol-2-one, 1-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-1,3-dihydro-3-[4-[[1,3,3,3-tetrafluoro-2-(4-methylphenyl)-1-propenyl]oxy]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844878-64-4 CAPLUS

CN 2-Imidazolidinone, 1-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-3-[4-[[1,3,3,3-tetrafluoro-2-(4-methylphenyl)-1-propenyl]oxy]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844878-65-5 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 2-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-4-[4-[[1-fluoro-2-(4-methoxyphenyl]ethenyl]oxy]phenyl]-2,4-dihydro- (CA INDEX NAME)

RN 844878-67-7 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 2-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-2,4-dihydro-4-[4-[[1,3,3,3-tetrafluoro-2-(4-methylphenyl)-1-propenyl]oxy]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844878-69-9 CAPLUS

CN 2H-Imidazol-2-one, 1-[4-[[2-(3,5-dichlorophenyl)-1,3,3,3-tetrafluoro-1-propenyl]oxy]phenyl]-3-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-1,3-dihydro- (9CI) (CA INDEX NAME)

RN 844878-71-3 CAPLUS

CN 2-Imidazolidinone, 1-[4-[[2-(3,5-dichlorophenyl)-1,3,3,3-tetrafluoro-1-propenyl]oxy]phenyl]-3-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844878-73-5 CAPLUS

CN 2H-Imidazol-2-one, 1-[4-[[2-(3-chlorophenyl)-1,3,3,3-tetrafluoro-1-propenyl]oxy]phenyl]-3-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-<math>3-(1H-1,2,4-triazol-1-yl)propyl]-1,3-dihydro-(9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

RN 844878-75-7 CAPLUS

CN 2-Imidazolidinone, 1-[4-[[2-(1,3-benzodioxol-5-yl)-1,3,3,3-tetrafluoro-1-propenyl]oxy]phenyl]-3-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]- (9CI) (CA INDEX NAME)

RN 844878-77-9 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 2-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-4-[4-[(1-fluoro-2-phenylethenyl)oxy]phenyl]-2,4-dihydro- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844878-79-1 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 2-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-4-[4-[[2-(4-ethylphenyl)-1-fluoroethenyl]oxy]phenyl]-2,4-dihydro- (CA INDEX NAME)

RN 844878-81-5 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 4-[4-[[2-(4-chlorophenyl)-1-fluoroethenyl]oxy]phenyl]-2-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-2,4-dihydro- (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

RN 844878-83-7 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 4-[4-[[2-(3-chlorophenyl)-1-fluoroethenyl]oxy]phenyl]-2-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-2,4-dihydro- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844878-85-9 CAPLUS

CN 2H-Imidazol-2-one, 1-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-3-[4-[(1-fluoro-2-phenylethenyl)oxy]phenyl]-1,3-dihydro- (CA INDEX NAME)

RN 844878-87-1 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 4-[4-[[2-(1,3-benzodioxol-5-yl)-1,3,3,3-tetrafluoro-1-propenyl]oxy]phenyl]-2-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-2,4-dihydro-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844878-89-3 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 4-[4-[[2-(4-chlorophenyl)-1,3,3,3-tetrafluoro-1-propenyl]oxy]phenyl]-2-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-2,4-dihydro- (9CI) (CA INDEX NAME)

RN 844878-90-6 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 4-[4-[[2-(3,4-dichlorophenyl)-1-fluoroethenyl]oxy]phenyl]-2-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-2,4-dihydro- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844878-92-8 CAPLUS

CN 2H-Imidazol-2-one, 1-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-3-[4-[[1-fluoro-2-(3-methylphenyl)ethenyl]oxy]phenyl]-1,3-dihydro- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844878-94-0 CAPLUS

CN 2H-Imidazol-2-one, 1-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-1,3-dihydro-3-[4-[[1,3,3,3-tetrafluoro-2-(4-methoxyphenyl)-1-propenyl]oxy]phenyl]- (9CI) (CA INDEX NAME)

RN 844878-96-2 CAPLUS

CN 2-Imidazolidinone, 1-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-3-[4-[(1-fluoro-2-phenylethenyl)oxy]phenyl]-(CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844878-98-4 CAPLUS

CN 2H-Imidazol-2-one, 1-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-3-[4-[[2-(4-ethylphenyl)-1-fluoroethenyl]oxy]phenyl]-1,3-dihydro- (CA INDEX NAME)

RN 844879-02-3 CAPLUS

CN 2-Imidazolidinone, 1-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-3-[4-[[2-(4-ethylphenyl)-1-fluoroethenyl]oxy]phenyl]- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844879-05-6 CAPLUS

CN 2H-Imidazol-2-one, 1-[4-[[2-(4-chlorophenyl)-1-fluoroethenyl]oxy]phenyl]-3-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-1,3-dihydro- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844879-08-9 CAPLUS

CN 2-Imidazolidinone,  $1-[4-[[2-(4-\text{chlorophenyl})-1-\text{fluoroethenyl}] \circ xy] \text{phenyl}]-3-[(1R,2R)-2-(2,4-\text{difluorophenyl})-2-\text{hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl}]- (CA INDEX NAME)$ 

RN 844879-11-4 CAPLUS

CN 2H-Imidazol-2-one, 1-[4-[[2-(3-chlorophenyl)-1-fluoroethenyl]oxy]phenyl]-3-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-1,3-dihydro- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

RN 844879-13-6 CAPLUS

CN 2-Imidazolidinone, 1-[4-[[2-(3-chlorophenyl)-1-fluoroethenyl]oxy]phenyl]-3[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1yl)propyl]- (CA INDEX NAME)

RN 844879-15-8 CAPLUS

CN 2H-Imidazol-2-one, 1-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-3-[4-[[1-fluoro-2-(3-fluorophenyl)ethenyl]oxy]phenyl]-1,3-dihydro- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844879-17-0 CAPLUS

CN 2-Imidazolidinone, 1-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-3-[4-[[1-fluoro-2-(3-fluorophenyl)ethenyl]oxy]phenyl]- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844879-19-2 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 2-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-2,4-dihydro-4-[4-[(1,3,3,3-tetrafluoro-2-phenyl-1-propenyl)oxy]phenyl]- (9CI) (CA INDEX NAME)

RN 844879-21-6 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 2-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-2,4-dihydro-4-[4-[[1,3,3,3-tetrafluoro-2-(3-methylphenyl)-1-propenyl]oxy]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844879-23-8 CAPLUS

CN 3H-1,2,4-Triazol-3-one, 4-[4-[[2-(3-chlorophenyl)-1,3,3,3-tetrafluoro-1-propenyl]oxy]phenyl]-2-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-2,4-dihydro- (9CI) (CA INDEX NAME)

RN 844879-25-0 CAPLUS

CN 2H-Imidazol-2-one, 1-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-1,3-dihydro-3-[4-[(1,3,3,3-tetrafluoro-2-phenyl-1-propenyl)oxy]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844879-26-1 CAPLUS

CN 2-Imidazolidinone, 1-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-3-[4-[(1,3,3,3-tetrafluoro-2-phenyl-1-propenyl)oxy]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844879-28-3 CAPLUS

CN 2H-Imidazol-2-one, 1-[4-[[2-(1,3-benzodioxol-5-yl)-1,3,3,3-tetrafluoro-1-propenyl]oxy]phenyl]-3-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-1,3-dihydro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844879-30-7 CAPLUS

CN 2-Imidazolidinone,  $1-[4-[[2-(3-\text{chlorophenyl})-1,3,3,3-\text{tetrafluoro}-1-\text{propenyl}] \circ xy] phenyl] -3-[(1R,2R)-2-(2,4-\text{difluorophenyl})-2-\text{hydroxy}-1-\text{methyl}-3-(1H-1,2,4-\text{triazol}-1-yl) propyl]- (9CI) (CA INDEX NAME)$ 

Absolute stereochemistry.

Double bond geometry unknown.

RN 844879-32-9 CAPLUS

CN 2H-Imidazol-2-one, 1-[4-[[2-(4-chlorophenyl)-1,3,3,3-tetrafluoro-1-propenyl]oxy]phenyl]-3-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-<math>3-(1H-1,2,4-triazol-1-yl)propyl]-1,3-dihydro-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

RN 844879-34-1 CAPLUS

CN 2H-Imidazol-2-one, 1-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-1,3-dihydro-3-[4-[[1,3,3,3-tetrafluoro-2-(3-methoxyphenyl)-1-propenyl]oxy]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844879-36-3 CAPLUS

CN 2H-Imidazol-2-one, 1-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-3-[4-[[1-fluoro-2-(3-methoxyphenyl)ethenyl]oxy]phenyl]-1,3-dihydro- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844879-38-5 CAPLUS

CN 2H-Imidazol-2-one, 1-[4-[[2-(1,3-benzodioxol-5-yl)-1-fluoroethenyl]oxy]phenyl]-3-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-1,3-dihydro- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844879-41-0 CAPLUS

CN 2H-Imidazol-2-one, 1-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-3-[4-[[1-fluoro-2-(4-methylphenyl)ethenyl]oxy]phenyl]-1,3-dihydro- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844879-44-3 CAPLUS

CN 2-Imidazolidinone,  $1-[4-[[2-(4-\text{chlorophenyl})-1,3,3,3-\text{tetrafluoro}-1-\text{propenyl}] \circ xy] phenyl] -3-[(1R,2R)-2-(2,4-\text{difluorophenyl})-2-\text{hydroxy}-1-\text{methyl}-3-(1H-1,2,4-\text{triazol}-1-yl) propyl]- (9CI) (CA INDEX NAME)$ 

Absolute stereochemistry. Double bond geometry unknown.

RN 844879-46-5 CAPLUS

CN 2-Imidazolidinone, 1-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-3-[4-[[1,3,3,3-tetrafluoro-2-(3-methoxyphenyl)-1-propenyl]oxy]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844879-48-7 CAPLUS

CN 2-Imidazolidinone, 1-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-3-[4-[[1-fluoro-2-(3-methoxyphenyl)ethenyl]oxy]phenyl]- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844879-50-1 CAPLUS

CN 2-Imidazolidinone, 1-[4-[[2-(1,3-benzodioxol-5-yl)-1-fluoroethenyl]oxy]phenyl]-3-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 844879-53-4 CAPLUS

CN 2-Imidazolidinone, 1-[(1R,2R)-2-(2,4-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-3-[4-[[1-fluoro-2-(4-methylphenyl)ethenyl]oxy]phenyl]- (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L89 ANSWER 1 OF 36 MARPAT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 148:262617 MARPAT Full-text

TITLE: Preparation of pyrimidine- and triazine-derivative

endothelin receptor antagonists

INVENTOR(S): Riechers, Hartmut; Klinge, Dagmar; Amberg, Wilhelm;

Kling, Andreas; Mueller, Stefan; Baumann, Ernst; Rheinheimer, Joachim; Vogelbacher, Uwe Josef; Wernet,

Wolfgang; Unger, Liliane; Raschack, Manfred

PATENT ASSIGNEE(S): Abbott Gmbh & Co. KG, Germany

SOURCE: U.S., 18pp., Cont. of U.S. Ser. No. 748,184.

CODEN: USXXAM

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

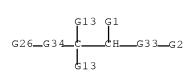
PATENT NO. KIND DATE APPLICATION NO. DATE

									_	
	7109205				US 2	2003-60	2275	2003062	4	
US	20040092742	A1 2	0040513							
DE	19533023	A1 1	9960418		DE 1	.995-19	533023	1995090	7	
	19533023									
WO	9611914	A1 1	9960425		WO 1	995-EP	3963	1995100	7	
	W: AU, BG,	, BR, BY,	CA, CN,	CZ,	FI, HU	J, JP,	KR, KZ	, MX, NO	NZ,	PL,
	RU, SG,	, SI, SK,	UA, US							
	RW: AT, BE,	CH, DE,	DK, ES,	FR,	GB, GR	R, IE,	IT, LU	, MC, NL	PT,	SE
EP	1110952	A1 2	0010627		EP 2	2001-10	3889	1995100	7	
EP	1110952	B1 2	0040929							
	R: AT, BE,	CH, DE,	DK, ES,	FR,	GB, GR	R, IT,	LI, LU	, NL, SE	PT,	ΙE
US	5932730	A 1	9990803		US 1	997-80	9699	1997032	7	
US	5969134	A 1	9991019		US 1	998-18	4152	1998110	2	
US	6197958	B1 2	0010306		US 1	.999-30	9770	1999051	1	
US	20020052495	A1 2	0020502		US 2	2000-74	8184	2000122	7	
US	6600043	B2 2	0030729							
US	20060160808	A1 2	0060720		US 2	2006-37	7879	2006031	5	
US	7119097	B2 2	0061010							
US	20060276645	A1 2	0061207		US 2	2006-50	2257	2006081	)	
US	20060276474	A1 2	0061207		US 2	2006-50	2293	2006081	)	
US	20070203338	A1 2	0070830		US 2	2007-78	9630	2007042	5	
PRIORIT	Y APPLN. INFO	D.:			DE 1	994-44	36851	1994101	4	
					DE 1	995-19	533023	1995090	7	
					WO 1	995-EP	3963	1995100	7	
					US 1	997-80	9699	1997032	7	
					US 1	998-18	4152	1998110	2	
					US 1	.999-30	9770	1999051	1	
					US 2	2000-74	8184	2000122	7	
					EP 1	.995–93	5916	1995100	7	
					US 2	003-60	2275	2003062	4	
					US 2	2006-50	2257	2006081	)	
СТ										

GI

The title compds. I [R = CHO, tetrazolyl, CN, CO2H, groups cleavable to CO2H; R2 = (un)substituted NH2, halogen, (un)substituted alkyl, etc.; R3 = H, OH, (un)substituted NH2, halogen, (un)substituted alkyl, etc.; R4, R5 = (un)substituted Ph or naphthyl; R6 = H, alkyl, alkenyl, alkynyl, alkylcarbonyl, (un)substituted Ph, etc.; X = N, (un)substituted CH; Y = direct bond, S, O; Z = S, O, SO, SO2, direct bond], and their pharmaceutically acceptable salts, are prepared and disclosed as endothelin receptor antagonists. In receptor binding assays, pyrimidine derivative II (R2 and R3 = MeO), m.p. 167°, demonstrated a Ki ETA of 6 nM. In particular, the racemate and individual enantiomers of II (R2 and R3 = Me) are claimed.

MSTR 1A



G1 = tetrazolyl

G13 = Ph (opt. substd. by 1 or more G14)

G14 = halo

G26 = carbon chain <containing 1-8 C,

0 or more double bonds, 0 or more triple bonds>

(opt. substd. by G27)

G27 = halo / Ph (opt. substd. by 1 or more G28)

G33 = 0 G34 = 0

Patent location: disclosure

Note: substitution is restricted

REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L89 ANSWER 2 OF 36 MARPAT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 147:9932 MARPAT Full-text

TITLE: Preparation of pyrimidinyl-oxy-propionates and related

compounds as endothelin antagonists

INVENTOR(S): Amberg, Wilhelm; Baumann, Ernst; Hergenroeder, Stefan;

Kling, Andreas; Klinge, Dagmar; Raschack, Manfred; Riechers, Hartmut; Schult, Sabine; Unger, Liliane

PATENT ASSIGNEE(S): Germany

SOURCE: Hung. Pat. Appl., 51pp.

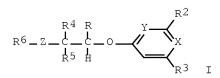
CODEN: HUXXCV

DOCUMENT TYPE: Patent LANGUAGE: Hungarian

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
HU 9903371	A2	20000228	ни 1999-3371	19970404
HU 9903371	A3	20000428		
PRIORITY APPLN.	INFO.:		HU 1999-3371	19970404
GI				



AB Pyrimidinyl-oxy-propionates I, wherein R is a group that can be hydrolyzed into a tetrazolyl, nitrile, carboxy; R2 is H, halogen, OH, NH2, NH(alkyl),

N(alkyl)2, alkyl, halogen-alkyl, alkoxy, halogen-alkoxy, alkyl-thio; or it forms a 5 or 6-member ring with CR2; X = N, substituted C; Y is N or CH; Z is O, S; R3 is H, halogen, OH, NH2, NH(alkyl), N(alkyl)2, alkyl, halogen-alkyl, alkoxy, halogen-alkoxy, alkoxy-amino, alkyl-thio; or it forms a 5 or 6 member ring with CR3; R4, R5 in a certain case, is Ph or a substituted Ph or naphthyl; naphthyl that are connected to each other in ortho position through a chemical bond, -CH2-, -CH2-CH2-, -CH=CH-, -SO2-, -NH-, -N(alkyl)-, -O- or -S-; cycloalkyl; R6 is H, alkyl, alkenyl, alkynyl, cycloalkyl, Ph, naphthyl, 5 or 6 member heteroaryl, were prepared as endothelin receptor inhibitors. Thus, Me 2-hydroxy-3-methoxy-3,3- diphenyl-propionate was prepared and reacted with 2,6-dimethoxy-4-chloro- pyrimidine, and K2CO3 at 100 °C in DMF to give Me 2-(2,6-dimethoxy-pyrimidin-4-yl-oxy)-3-methoxy-3,3-diphenyl-propionate. I bound to endothelin ETA receptors with Ki = 0.038 - 3.3  $\mu$ M.

MSTR 1

$$G45 - G44 - C - CH - O - G8$$

G1 = tetrazolyl

G40 = Ph (opt. substd. by 1 or more G41)

G41 = halo

G44 = O

G45 = alkenyl <containing 3-6 C>

(opt. substd. by 1 or more G46)

G46 = halo / Ph (opt. substd. by 1 or more G51)

Patent location: claim 1

Note: additional ring formation also claimed

L89 ANSWER 3 OF 36 MARPAT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 146:477108 MARPAT Full-text

TITLE: Preparation of dialkylpyridoazines as agricultural

fungicides

INVENTOR(S): Dietz, Jochen; Grammenos, Wassilios; Huenger, Udo;

Lohmann, Jan Klaas; Renner, Jens; Rheinheimer, Joachim

PATENT ASSIGNEE(S): BASF A.-G., Germany SOURCE: Ger. Offen., 51pp.
CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

----DE 102005051514 A1 20070503 DE 2005-10200505151420051026
PRIORITY APPLN. INFO.: DE 2005-10200505151420051026
GI

AB Title compds. [I; R1 = (substituted) alkyl, alkoxyalkyl, alkoxyalkenyl, alkoxyalkynyl, cycloalkyl, Ph, phenylalkyl, alkenyl, alkynyl; R2 = (substituted) alkyl, alkenyl, alkynyl; W, X, Y, Z = ≤3 N, CR3; R3 = H, halo, alkyl, alkoxy], were prepared for control of plant pathogenic fungi (no data).

MSTR 1

$$\text{GT}_{\text{G4}}^{\text{G1}}$$

$$G1 = 127$$

G2 = F / CN / OH / Ph (opt. substd. by (1-4) G3)

G3 = F

G13 = alkenylene < containing 2-12 C>

(opt. substd. by (1-3) G2)

G15 = alkyl <containing 1-6 C> (opt. substd. by (1-3) G2)

Patent location: claim 1

Note: also incorporates claim 8, structures 5a and 6a

MSTR 3

$$H_2 \subset G^1$$

$$G1 = 127$$

```
10/566911
    = F / CN / OH / Ph (opt. substd. by (1-4) G3)
G2
G3
    = F
G13 = alkenylene <containing 2-12 C>
       (opt. substd. by (1-3) G2)
G15 = alkyl <containing 1-6 C> (opt. substd. by (1-3) G2)
Patent location: claim 5
 MSTR 4
G1 = 127
1913—0—G15
G2 = F / CN / OH / Ph (opt. substd. by (1-4) G3)
G3
    = F
G13 = alkenylene <containing 2-12 C>
      (opt. substd. by (1-3) G2)
G15 = alkyl < containing 1-6 C > (opt. substd. by (1-3) G2)
                claim 5
Patent location:
MSTR 5
 G1____G7
G1 = 127
1273—0—G15
G2 = F / CN / OH / Ph (opt. substd. by (1-4) G3)
G3
     = F
G13 = alkenylene <containing 2-12 C>
```

MSTR 9

Patent location:

(opt. substd. by (1-3) G2)

= alkyl <containing 1-6 C> (opt. substd. by (1-3) G2)

claim 5

$$G1 = 127$$

1613—0—G15

MSTR 10

$$\operatorname{GT}^{0}_{\operatorname{NH}_{2}}\operatorname{CH}_{2}\operatorname{-G1}$$

$$G1 = 127$$

MSTR 12

$$\begin{array}{c} G & \xrightarrow{\text{CH}_2-\text{G1}} \\ G & \xrightarrow{\text{NH}-\text{C}-\text{G4}} \end{array}$$

```
G1
    = 127
1913—0—G15
      = F / CN / OH / Ph (opt. substd. by (1-4) G3)
G2
G3
      = F
G13
      = alkenylene <containing 2-12 C>
       (opt. substd. by (1-3) G2)
      = alkyl <containing 1-6 C> (opt. substd. by (1-3) G2)
G15
                     claim 8
Patent location:
L89 ANSWER 4 OF 36 MARPAT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 145:418786 MARPAT Full-text
TITLE:
                        Substituted benzylamines as CYP2A inhibitors and their
                        preparation and use in treatment of nicotine
                        dependence
                        Ghosheh, Omar; Raymond, Jeff
INVENTOR(S):
                       Inflazyme Pharmaceuticals Ltd., Can.; Roth, Carol, J.
PATENT ASSIGNEE(S):
SOURCE:
                        PCT Int. Appl., 68pp.
                        CODEN: PIXXD2
DOCUMENT TYPE:
                        Patent
LANGUAGE:
                        English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:
    PATENT NO. KIND DATE
                                        APPLICATION NO. DATE
    WO 2006108149 A2 20061012
WO 2006108149 A3 20071122
                                        WO 2006-US13081 20060406
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
            CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
            GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR,
            KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX,
            MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE,
            SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC,
            VN, YU, ZA, ZM, ZW
        RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
            IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
            CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
            GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
            KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA
    EP 1871357 A2 20080102 EP 2006-740741 20060406
        R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
            IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL,
            BA, HR, MK, YU
PRIORITY APPLN. INFO.:
                                          US 2005-669038P 20050406
                                          WO 2006-US13081 20060406
GΙ
```

85

$$R^{3}$$
  $4 = 5 - 6 - 7 - N - R^{1}$   $F_{3}C$   $N = 1$   $K^{2}$   $K^{2}$ 

AΒ This invention is directed to substituted benzylamines of formula I which are useful as inhibitors of the CYP2A6 enzyme. Pharmaceutical compns. comprising the compds. and methods of using the compds. to treat nicotine dependence are also disclosed. Compds. of formula I wherein R1 and R2 are independently H, (un) substituted aryl, (un) substituted cycloalkyl, (un) substituted C1-30 alkyl; R1R2 together with the N they are attached may form an (un)substituted heterocyclyl; R3 is X, (un)substituted C1-30 (halo)alkyl, NO2, carboxy, SO2R, and SO2NR2; R4 is H, X, (un)substituted C1-30 (halo)alkyl, OR, SR, NR2; R2R4 together with the N they are attached to may form an (un)substituted fused heterocycle; numerals 1 - 7 is carbon atoms; numerals 2, 3 and 5 are independently optionally substituted with X, R, NR2 and OR; numeral 7 is optionally substituted with =0, =CR2, =C=CR2, CR2(CR2)n and O(CR2)nO; X is F, Br, Cl and I; R is H and C1-30 organic moiety; and their stereoisomers, mixts. of stereoisomers, pharmaceutically acceptable salts, solvates, and prodrugs thereof are claimed. Example compound II was prepared by amidation of 3trifluoromethylbenzoyl chloride with cyclopentylamine; the resulting Ncyclopentyl-3-trifluoromethylbenzamide underwent reduction to give compound II. All the invention compds. were evaluated for their CYP2A inhibitory activity. The most potent compds. of the invention showed greater than 98% inhibition.

MSTR 1

G3 = F G5 = F G6 = 93

G9 = carbon chain <containing 1-30 C, 0 or more double bonds> (opt. substd. by G26) G13 = 2-10 3-41 1-43 6-42

G20 = OH / 99

98----G9

G26 = F / Ph

Patent location: claim 1

Note: or mixtures or pharmaceutically acceptable salts,

solvates, and prodrugs, or pharmaceutically acceptable carriers, diluents, or excipients

Stereochemistry: and stereoisomers

L89 ANSWER 5 OF 36 MARPAT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 144:211234 MARPAT Full-text

TITLE: Chemoenzymic process for synthesis of of

cis-configured 3-hydroxycyclohexane carboxylic acid

derivative enantiomers

INVENTOR(S): Holla, Wolfgang; Keil, Stefanie; Tappertzhofen,

Christoph

PATENT ASSIGNEE(S): Sanofi-Aventis Deutschland GmbH, Germany

SOURCE: PCT Int. Appl., 77 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PAT	TENT	NO.		KI	ND	DATE		APPLICATION NO. DATE									
	2006 2006								M	D 20	 05-Е	 P805	8	2005	0723		
								Α7	BA.	BB.	BG.	BR.	BW.	BY,	B7.	CA.	CH.
	•••					•							•	ES,			•
						•						•	•	KM,			•
		•				•	•		•		•			MW,			•
		•	•			•								SD,		•	
					IJ,	ΤМ,	IN,	IK,	ΙΙ,	12,	UA,	UG,	05,	UZ,	VC,	VN,	ĭυ,
		,	ZM,		~	~	~ =							~-	~-		
	RW:													GB,			
		IS,	ΙΤ,	LT,	LU,	LV,	MC,	ΝL,	PL,	PT,	RO,	SE,	SI,	SK,	TR,	BF,	ВJ,
		CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	ΝE,	SN,	TD,	ΤG,	BW,	GH,
		GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	AΖ,	BY,
		KG,	KΖ,	MD,	RU,	ТJ,	TM										
DE	1020	0403	8403	А	1	2006	0223		D:	E 20	04-1	0200	4038	34032	0040	807	
DE	1020	0403	8403	В	4	2006	0831										
AU	2005	2704	47	А	1	2006	0216		A	U 20	05-2	7044	7	2005	0723		
CA	2576	080		А	1	2006	0216		C	A 20	05-2	5760	80	2005	0723		
	1989					2007				_				2005	-		
	1805									_					-		
111														GB,		ווט	TE
	1/	$\Delta_{\perp}$ ,	DE,	DG,	$C\Pi$ ,	$\cup_{\perp}$ ,	$\cup \Delta$ ,	DE,	DK,	, دو	щO,	гт,	r r,	GD,	Gr,	110,	тс,

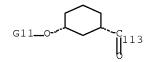
```
IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR
    JP 2008509102 T 20080327 JP 2007-524225 20050723
    MX 200700996
                   A
                        20070416
                                      MX 2007-996
                                                      20070125
    US 20070197788
                   A1 20070823
                                      US 2007-669545 20070131
    KR 2007041564
                   А
                        20070418
                                      KR 2007-702917
                                                     20070206
    IN 2007CN00548
                    Α
                         20070824
                                       IN 2007-CN548
                                                      20070207
PRIORITY APPLN. INFO.:
                                       DE 2004-10200403840320040807
                                       WO 2005-EP8058 20050723
```

AB The invention relates to a method for producing chiral, non-racemic, cisconfigured cyclohexanols or cyclohexanol derivs. by means of enzyme catalyzed kinetic resolution of racemates.

MSTR 3

G 8\_\_\_\_G 1

G8 = 113



G11 = 117

G12 = F / CF3 / CN / Ph (opt. substd. by (1-3) G14) / alkoxycarbonyl <containing 1-4 C>

(opt. substd. by (1-3) G14) / alkenyloxycarbonyl <containing 2-4 C> (opt. substd. by (1-3) G14)

G14 = F

G15 = carbon chain <containing 1-14 C,

0 or more double bonds, 0 or more triple bonds>

(opt. substd. by 1 or more G12)

Patent location: claim 1

Note: additional oxygen interruptions of Ak in G15 also

claimed

L89 ANSWER 6 OF 36 MARPAT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 143:78086 MARPAT Full-text

TITLE: Preparation of urea/carbamate derivatives as

inhibitors of coagulation factor Xa for treatment of

thromoboembolic disorders

INVENTOR(S): Cezanne, Bertram; Dorsch, Dieter; Mederski, Werner;

Tsaklakidis, Christos; Gleitz, Johannes

PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Germany

SOURCE: PCT Int. Appl., 80 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

			KIND DATE					APPLICATION NO. DATE									
	2005													2004	1119		
	W:	ΑE,	AG,	AL,	ΑM,	AT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FΙ,	GB,	GD,
		GE,	GH,	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KΕ,	KG,	KP,	KR,	KΖ,	LC,
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NΙ,
		NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,
				•		•	•		•					YU,	•		
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	ΑM,
		AΖ,	BY,	KG,	KZ,	MD,	RU,	ТJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	IS,	ΙT,	LU,	MC,	NL,	PL,	PT,	RO,
		SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,
		•		TD,													
	1035																
	2004																
	2549																
EP	1694	643		A.	1	2006	0830		E.	P 20	04 - 8	2005	3	2004	1119		
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙΤ,	LI,	LU,	NL,	SE,	MC,	PT,
		,	•		•					•	•		,	PL,		IS	
	1890																
	2004																
	2007																
	2006																
	2006													2006			
	2007				1	2007	0531							2006			
RIORIT	Y APP	LN.	INFO	.:										2003	_		
										0 20	04-E	P132	02	2004	1119		
THER SO	HER SOURCE(S):				CAS	REAC'	T 143	3:78	086								

GΙ

Title compds. I [D = halo, alkoxy, etc.; X = amino, O; Y = O, S, amino, etc.; R1 = H, aryl, heteroaryl, etc.; E = CH, N; Z, Z' = acyl, etc.; Q = O, amino, acyl, etc.; R4-4' = A, OH, alkoxy; T = (hetero)cyclyl, etc.] are prepared For instance, (R)-N-(4-chlorophenyl)-N'-[2-[4-(4-fluorophenyl)piperazin-1-yl]-2-oxo-1-phenylethyl]urea (II) is prepared in 3 steps from 1-methyl-4,4'-bipiperidinyl, (R)-N-(tert-butoxycarbonyl)phenylglycine and 4-chlorophenylisocyanate. II has IC50 = 6 x 10-9 M for Factor Xa. I are inhibitors of coagulation factor Xa and can be used for the prophylaxis and/or the treatment of thromboembolic diseases and for treating tumors.

MSTR 1

G3 = 0 = Ph (opt. substd. by G34) G4G9 = (1-4) CH2 = (0-4) CH2 G10 = NG11 G12 = Ph (opt. substd. by G30) = carbon chain <containing 1 or more C, G19 0 or more double bonds, no triple bonds> (opt. substd. by 1 or more G20) G20 = F / PhG30 = 73

79----G19

$$G33 = 88-6 90-33$$



G34 = F G41 = 301



G42 = 4

Patent location: claim 1

Note: also incorporates claim 22, formulae II and IV

Note: substitution is restricted

Note: or pharmaceutically acceptable salts, solvates, and

derivatives

Note: additional substitution also claimed Stereochemistry: and stereoisomers and derivatives

REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L89 ANSWER 7 OF 36 MARPAT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 143:26591 MARPAT Full-text

TITLE: Preparation of benzoxazoles or benzothiazoles as

fungicides

INVENTOR(S): Hara, Yoshihiko; Sano, Hiroshi; Haramoto, Masanori

PATENT ASSIGNEE(S): Nippon Soda Co., Ltd., Japan SOURCE: Jpn. Kokai Tokkyo Koho, 40 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2005145840	A	20050609	JP 2003-382721	20031112
PRIORITY APPLN. INFO.	:		JP 2003-382721	20031112
GI				

X1 NH—R2

AB Title compds. I [R1 = H, C1-4 alkyl, OH, etc.; R2 = AB, YCOZ; A = single bond, (substituted) C1-6 alkylene; B = (substituted) Ph, (substituted) naphthyl, etc.; Y = (substituted) C1-6 alkylene; Z = OR3, NR3R4; R3 = (substituted) C1-16 alkyl, (substituted) C3-10 cycloalkyl, etc.; R2R3 may form ring; X1, X2 = O, S; substituents for A, B, Y, and R3 are given] are prepared Thus, N-(1-ethyloxycarbonyl-2,2-dimethylpropyl)-2-hydroxy-3- nitrobenzamide was reduced over Pd/C and condensed with tri-Et orthoformate to give 95% I (R1 = H, R2 = 1-ethyloxycarbonyl-2,2-dimethylpropyl, X1 = X2 = O).

MSTR 1

```
10/566911
```

G3 = 171611—C(O)-G15 G4 = alkylene <containing 1-6 C> G11 (opt. substd. by 1 or more G12) = alkyl <containing 1-12 C> / G12 alkenyl <containing 2-8 C> (opt. substd. by 1 or more G6) / alkynyl <containing 2-8 C> (opt. substd. by 1 or more G6) / alkyl <containing 1-8 C> (substd. by 1 or more G13) / alkoxycarbonyl <containing 1-8 C> Ph (opt. substd. by 1 or more G4) = alkoxycarbonyl <containing 1-8 C> G13 alkylaminocarbonyl <containing 1-8 C> G15 2620-G16 = alkenyl <containing 2-8 C> G16 (opt. substd. by 1 or more G18) = Ph (opt. substd.) / F G18 G20 = 0Patent location: claim 1 L89 ANSWER 8 OF 36 MARPAT COPYRIGHT 2008 ACS on STN 142:240437 MARPAT Full-text ACCESSION NUMBER: TITLE: Preparation of triazolylmethanol derivatives as antifungal agents Kim, Bum Tae; Min, Yong Ki; Lee, Yeon Soo; Park, No INVENTOR(S): Kyun; Kim, Woo Jung PATENT ASSIGNEE(S): Korea Research Institute of Chemical Technology, S. Korea SOURCE: PCT Int. Appl., 58 pp. CODEN: PIXXD2 DOCUMENT TYPE: Patent English LANGUAGE: FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION: PATENT NO. KIND DATE APPLICATION NO. DATE \_\_\_\_\_ WO 2004-KR1996 20040809 WO 2005014583 A1 20050217 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,

```
PATENT NO. KIND DATE APPLICATION NO. DATE

WO 2005014583 A1 20050217 WO 2004-KR1996 20040809

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

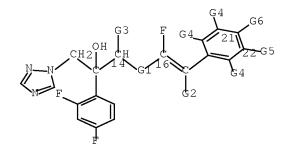
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
```

SN, TD, TG KR 2005017962 А 20050223 KR 2003-55590 20030812 EP 1654254 Α1 20060510 EP 2004-748524 20040809 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK JP 2007502268 20070208 JP 2006-523125 20040809 US 20080027117 Α1 20080131 US 2006-566911 20060203 PRIORITY APPLN. INFO.: KR 2003-55590 20030812 WO 2004-KR1996 20040809 OTHER SOURCE(S): CASREACT 142:240437

GΙ

Title compds. represented by the formula I [wherein A = 0, 1,2,4-triazolyl-AΒ PhO-, 1,2,4-triazolone-3-yl-PhO-, imidazolone-1-yl-PhO, imidazolinone-1-yl-PhO-; R = H or CF3; R' = H or alkyl; X = H, halo, (halo)alkyl,alkoxy, 3,4dioxyalkylene; and pharmaceutically acceptable salts, isomers or esters thereof] were prepared as antifungal agents for the treatment of humans or animals. For example, II was given in a multi-step synthesis starting from the reaction of Me (R)-lactate with morpholine. I showed antifungal activity in vivo against a wide spectrum of pathogenic fungi, such as ATCC 10231 and MYA-573, and low toxicity in oral administration.

MSTR 1



G1 = 0

Patent location: claim 1

Note: or pharmaceutically acceptable salts or esters

Stereochemistry: or isomers

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L89 ANSWER 9 OF 36 MARPAT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 142:225780 MARPAT Full-text

TITLE: Pharmaceutical compositions containing amino alcohol

derivatives or phosphonic acid derivatives for use as

immunosuppressants

INVENTOR(S): Nishi, Takehide; Shimozato, Ryuichi; Nara, Futoshi;

Miyazaki, Shojiro

PATENT ASSIGNEE(S): Sankyo Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 253 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	API	PLICATION NO.	DATE
JP 2005041867	A	20050217	JP	2004-197492	20040705
US 20070105933	A1	20070510	US	2006-636776	20061211
PRIORITY APPLN. INFO.	:		JP	2003-193599	20030708
			JP	2002-4456	20020111
			JP	2002-4484	20020111
			WO	2003-JP136	20030109
			JP	2003-4599	20030110
			JP	2004-197492	20040705
			US	2004-889657	20040712

GΙ

$$R^{3}$$
0  $R^{4}$   $(CH_{2})$   $n$   $R^{6}$   $R^{7}$   $Y-Z-R^{5}$   $I$ 

AΒ The invention relates to pharmaceutical compns. for use as immunosuppressants for treatment and/or prevention of rheumatoid arthritis, Crohn's disease, ulcerative colitis, multiple sclerosis, psoriasis vulgaris, atopic dermatitis, insulin-dependent diabetes, glomerulonephritis, and graft rejection, etc., characterized by containing alc. derivs. or phosphonic acid derivs. I [R1, R2 = H, lower alkyl, an amino-protecting group; R3 = H, lower alkyl, a hydroxyprotecting group; R4 = lower alkyl; n = 1-6; X = 0, (un) substituted N; Y =ethylene, vinylene, ethynylene, COCH2, CH(OH)CH2, (un)substituted C6-10 arylene; Z = a single bond, C1-10 (un)substituted alkylene optionally containing O or S in or at terminus of the carbon chain; R5 = H, each (un) substituted C3-10 cycloalkyl, C6-10 aryl, 5-7-membered heterocyclyl containing 1-3 of S, O, and/or N; R6, R7 = H, halo, lower alkyl, lower haloalkyl, lower alkoxy, lower alkylthio, CO2H, lower alkoxycarbonyl, HO, lower aliphatic acyl, NH2, mono- or di(lower alkyl) amino, lower aliphatic acylamino, cyano, NO2; provided that when R5 is hydrogen, then Z is branched or substituted C1-10 alkylene or C1-10 alkylene containing O or S in or at terminus of the carbon chain], pharmacol. acceptable salts thereof or pharmacol. acceptable esters thereof. For example, a compound (2R)-2-amino-2methyl-4-[5-(5- cyclohexylpent-1-ynyl)furan-2-yl]butan-1-ol was prepared, and its effect on adjuvant arthritis rats was examined

MSTR 1

$$G7 = 18-4 \ 19-6 \ / \ 30-4 \ 32-6 \ / \ 38-4 \ 40-6 \ / \ 43-4 \ 44-6 \ / \ 45-4 \ 46-6$$

$${}_{1} \underbrace{ \{8 - 1\}^{13} }_{3} \underbrace{ \{6 \}^{14} \underbrace{ \{4 \}^{15} }_{3} \underbrace{ \{1 \}^{16} }_{3} \underbrace{ \{3 \}^{19} \underbrace{ - G15}_{4} \underbrace{ \{6 \}^{18} }_{4} \underbrace{ \{4 \}^{20} \underbrace{ \{4 \}^{15} }_{4} \underbrace{ \{4 \}^{25} }_{4} \underbrace{ \{4 \}^{$$

25(0)-G11

G13 = 35-18 37-6 / 41-18 42-6  

$$_{3}$$
 $_{6}$  $_{17}$ - $_{615}$  $_{3}$  $_{718}$   $_{4}$  $_{616}$  $_{4}$  $_{2}$  $_{15}$ 

G15 = 0

G18 = alkylene <containing 1-9 C>

(opt. substd. by (1-3) G12)

G21 = phenylene (opt. substd. by (1-3) G39)

G22 = Ph

G25 = 92-45 94-6 / 95-45 96-6

9618—G15—G18 9616—615

G39 = F

Patent location: claim 1

Note: or pharmacologically acceptable salts or esters Note: additional heteroatom interruptions also claimed

Note: substitution is restricted
Note: also incorporates claim 4 and 7

L89 ANSWER 10 OF 36 MARPAT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 140:406954 MARPAT Full-text

TITLE: Preparation of thienylalkyl phosphates or

(thienylalkyl)phosphonic acids as immunosuppressants

with low toxicity

INVENTOR(S): Nishi, Takehide; Shimozato, Ryuichi; Nara, Futoshi

PATENT ASSIGNEE(S): Sankyo Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 199 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004137208	A	20040513	JP 2002-304196	20021018
PRIORITY APPLN. INFO.	:		JP 2002-304196	20021018
GI				

AB The title compds. I [R1, R2 = H, lower aliphatic acyl, lower alkoxycarbonyl; R3, R8 = H, protecting group; R4 = H, lower (hydroxy)alkyl; n = 1-6; X = ethylene, vinylene, ethynylene, C6-10 arylene, etc.; Y = bond, C1-10 (un)substituted alkylene; Z = O, CH2; R5 = H, (un)substituted C3-10 cycloalkyl, (un)substituted C6-10 aryl, (un)substituted heterocyclyl; when R5 = H, then Y ≠ bond; R6, R7 = H, halo, lower (halo)alkyl, lower alkoxy, OH, cyano, NO2, etc.], their pharmacol. acceptable salts, or esters are prepared Thus, treatment of bis(allyl) mono[(2R)-tert- butoxycarbonylamino-2-methyl-4-[5-(5-phenylpentanoyl)thiophen-2-yl]butyl] phosphate with

tetrakis(triphenylphosphine)palladium gave 69% mono[(2R)-amino-2-methyl-4-[5-(5-phenylpentanoyl)thiophen-2-yl]butyl] phosphate, which inhibited host vs. graft reaction in rats with ID50 value of 0.0878 mg/kg.

MSTR 1

$$G3 = \frac{1}{G_3} G40 = CH_2 = \frac{G^1}{G_5} G6 = \frac{G}{G^2} G7 = \frac{G}{G^2} G22$$

G22 = Ph G25 = 92-45 94-6 / 95-45 96-6

9618—G15<del>9</del>631 9628<del>9</del>615

 $_{3}$   $_{6}$   $_{1}$   $_{7}$   $_{-6}$   $_{1}$   $_{5}$   $_{3}$   $_{6}$   $_{1}$   $_{1}$   $_{1}$   $_{1}$   $_{2}$   $_{1}$   $_{2}$   $_{1}$   $_{2}$   $_{3}$   $_{1}$   $_{2}$   $_{3}$   $_{1}$   $_{2}$   $_{3}$   $_{2}$   $_{3}$   $_{2}$   $_{3}$   $_{2}$   $_{3}$   $_{2}$   $_{3}$   $_{2}$   $_{3}$   $_{2}$   $_{3}$   $_{2}$   $_{3}$   $_{2}$   $_{3}$   $_{2}$   $_{3}$   $_{2}$   $_{3}$   $_{2}$   $_{3}$   $_{2}$   $_{3}$   $_{2}$   $_{3}$   $_{2}$   $_{3}$   $_{2}$   $_{3}$   $_{3}$   $_{2}$   $_{3}$   $_{2}$   $_{3}$   $_{3}$   $_{2}$   $_{3}$   $_{3}$   $_{3}$   $_{2}$   $_{3}$ 

```
G31 = alkylene <containing 1-10 C>
(opt. substd. by (1-3) G12)
G39 = F
```

Patent location: claim 1

Note: or pharmacologically acceptable salts or esters additional heteroatom interruptions also claimed

Note: substitution is restricted Note: also incorporates claim 7

L89 ANSWER 11 OF 36 MARPAT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 139:197921 MARPAT Full-text

TITLE: Diol esters useful in preparation of a catalyst for olefin polymerization, process for preparing the same

and use thereof

INVENTOR(S): Gao, Mingzhi; Wang, Jun; Li, Changxiu; Li, Jiyu; Li,

Tianyi; Li, Xianzhong; Ma, Jing; Xing, Lingyan; Liu,

Haitao

PATENT ASSIGNEE(S): China Petroleum and Chemical Corp., Peop. Rep. China;

Beijing Research Institute of Chemical Industry; et

al.

SOURCE: PCT Int. Appl., 71 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

```
APPLICATION NO. DATE
    PATENT NO. KIND DATE
                                       _____
    WO 2003068723 A1 20030821 WO 2003-CN111 20030130
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
            CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
            GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
            LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
            PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ,
            UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
            KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
            FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF,
            BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
    CN 1436766 A 20030820 CN 2002-100896 20020207
    AU 2003245432
                    A1 20030904
                                      AU 2003-245432 20030130
                    A1 20041124 EP 2003-739422 20030130
    EP 1478617
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
    JP 2005517702 T 20050616
US 20050096389 A1 20050505
                                        JP 2003-567858 20030130
                                        US 2004-503119 20041201
PRIORITY APPLN. INFO.:
                                        CN 2002-100896 20020207
                                        WO 2003-CN111
                                                       20030130
```

The present application relates to diol ester compds. R1CO-O-CR3R4-A-CR5R6- O-AB CO-R2 (I; e.g. 1,2-ethylene glycol dibenzoate) wherein, R1 and R2 groups, which may be identical or different, can be (un) substituted hydrocarbyl having 1-20 C atoms, R3-R6 groups, which may be identical or different, can be H, halogen or (un)substituted hydrocarbyl having 1-20 C atoms, R1-R6 groups optionally contain ≥1 hetero-atoms replacing C, H atom or the both, said heteroatom = N, O, S, Si, P and halogen atom, two or more of R3-R6 groups can be linked to form saturated or unsatd. monocyclic or polycyclic ring; A is a single bond or bivalent linking group with chain length between two free radicals being 1-10 atoms, wherein said bivalent linking aliphatic, alicyclic and aromatic bivalent radicals, and can carry C1-C20 linear or branched substituents; ≥1 of C atom and/or H atom on the substituents can be replaced by a hetero-atom N, O, S, Si, P, and halogen atom, and two or more said substituents on the linking group as well as above-mentioned R3-R6 groups can be linked to form saturated or unsatd. monocyclic or polycyclic ring. I can be used as a electron donor compound in the preparation of a catalyst for

olefin polymerization, and a catalyst with excellent general properties can be obtained. When the catalyst obtained was used in polymerization of propylene, satisfactory polymerization yield was obtained, and stereo-direction of the polymer was very high. Even if an external donor is not used, relatively high isotactic polymer can still be obtained. Hydrogen response of the catalyst is excellent, and distribution of the mol. weight of the polymer obtained is relatively wide, and these properties are desirable in the development of different grades of polymers. In addition, when the catalyst is used in the copolymn. of olefins, especially in the copolymn. of ethylene and propylene, less gel content is achieved (no data). Ninety-nine example prepns. are included. For example, for preparation of 1,2-ethylene glycol dibenzoate (92 % yield), to 2.8 g (0.05 mol) 1,2-ethylene glycol was added 50 mL THF, then added 12.1ml (0.15 mol) pyridine with stirring. To the resulting homogeneous mixture was slowly added  $14.5 \, \text{mL}$  (0.125 mol) benzoyl chloride, and the mixture was stirred for 1 h at room temperature, then heated refluxing for 4 h. For preparation of the solid catalyst components, to a reactor which was completely replaced with high pure N2 were added successively 4.8 g MgCl2, 95 mL toluene, 4 mL epoxychloropropane, and 12.5 mL tri-Bu phosphate. The mixture was heated to  $50^{\circ}$  with stirring and held at the temperature for 2.5 h to dissolve the solid completely, then 1.4 g phthalic anhydride was added and the temperature was held for 1 h further. The solution was cooled to  $<-25^{\circ}$ and added dropwise were 56 mL TiCl4 over 1 h, then heating was slowly done to 80°; solid was precipitated gradually during the heating. To the system were added 6 mmol of diol ester and the reaction was held at the temperature with stirring for a further 1 h. After removing the supernatant, to the residue was added 70 mL toluene and the supernatant was removed again after mixing completely; the washing procedure was repeated twice. The resulting solid precipitate was treated with 60 mL toluene and 40 mL TiCl4 at 100° for 2 h, and after removing the supernatant, the residue was treated with 60 mL toluene and 40 mL TiCl4 at  $100^{\circ}$  for 2 h again. After removing the supernatant, the residue was washed with 60 mL toluene under boiling state for three times, 60 mL hexane under boiling state for two times, 60 mL hexane at normal temperature for two times to yield the solid catalyst components. The catalyst components obtained above were used in the polymerization of propylene. To a 5 L stainless steel autoclave, which had been replaced with propylene gas completely, were added 2.5 mmol AlEt3, 0.1 mmol cyclohexylmethyldimethoxysilane, .apprx.10 mg of the solid catalyst component prepared as above, and 1.2 L H2, followed by introduction of 2.3 L liquid propylene. The reactor was heated to 70°, and the polymerization was performed at that temperature and autogenous pressure for 1 h. In one case using 2,4-pentanediol bis(p-butylbenzoate) (22.1 weight % diol ester and 3.1 weight % Ti), 64.2 kg polypropylene/ g catalyst was obtained with 98.6 % isotacticity and a 9.7 mol. weight distribution.

MSTR 1

$$G1$$
— $C(0)$ — $g$ — $G2$ — $g$ — $C(0)$ — $G1$ 

$$G2 = 17-3 \ 19-5$$

```
G5
    = F / Ph (opt. substd. by G8)
G9
    = carbon chain <containing 1 or more C>
       (opt. substd. by G5) / 47
G10 = 0
Patent location: claim 1
MSTR 1
G1—C(0)—g—G2—g—C(0)—G1
G2 = 17-3 \ 19-5
169-G10-G9
G5 = F / Ph (opt. substd. by G8)
    = carbon chain <containing 1 or more C>
       (opt. substd. by G5) / 47
G10 = 0
Patent location: claim 1
MSTR 2
н9------ д н
G2 = 17-3 \ 19-5
199—G10—G9
```

G5 = F / Ph (opt. substd. by G8)

G8 = F

G9 = carbon chain <containing 1 or more C>
 (opt. substd. by G5) / 47

G 5—4G——G 5

G10 = 0

Patent location: claim 25

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L89 ANSWER 12 OF 36 MARPAT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 139:133462 MARPAT Full-text

TITLE: Preparation of 2-amino-4-(2-furanyl or

2-pyrrolyl)butanol or 3-amino-5-(2-furanyl or 2-pyrrolyl)pentylphosphonic acid derivatives as

immunosuppressants

INVENTOR(S): Nishi, Takahide; Shimozato, Takaichi; Nara, Futoshi;

Miyazaki, Shojiro

PATENT ASSIGNEE(S): Sankyo Company, Limited, Japan

SOURCE: PCT Int. Appl., 592 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PAI	ENT	NO.		KIND DATE				APPLICATION NO						DATE			
WO	2003	0598	80	A	1	2003	0724		M	20	: 03-J:	 P136		2003	0109		
	W:	ΑE,	AG,	AL,	ΑM,	AT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KP,	KR,	KΖ,	LC,	LK,	LR,
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,
		PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	ΤJ,	TM,	TN,	TR,	TT,	TZ,
		UA,	UG,	US,	UΖ,	VC,	VN,	YU,	ZA,	ZM,	ZW						
	RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	ΑM,	AZ,	BY,
		KG,	KΖ,	MD,	RU,	ТJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,
		FI,	FR,	GB,	GR,	HU,	IE,	ΙT,	LU,	MC,	NL,	PT,	SE,	SI,	SK,	TR,	BF,
		ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	$\mathrm{ML}_{m{\prime}}$	MR,	ΝE,	SN,	TD,	ΤG	
CA	2473	461		А	1	2003	0724		C.	A 20	03-2	4734	61	2003	0109		
														2003			
														2003			
EP														2003			
	R:	,	,	,	,	,	,	,	,	,	,	,	,	NL,	,	,	PT,
		,	,	,	,	,	,	,	,	,	,	,	,	EE,	,	SK	
_									_					2003			
														2003			
														2003			
														2004			
						2004								2004			
		0043		А		2005	_		U	S 20	04-8	8965	7	2004	0712		
	7199			В		2007											
						2004				-	-	-		2004			
ZA	2004	0063	33	A		2005	1020		$\mathbf{Z}_{\mathbf{z}}$	A 20	04-6	333		2004	0810		

US 20070105933	A1	20070510	US	2006-636776	20061211
US 20070142335	A1	20070621	US	2007-651205	20070109
PRIORITY APPLN. INFO.:			JP	2002-4456	20020111
			JP	2002-4484	20020111
			WO	2003-JP136	20030109
			JP	2003-4599	20030110
			JP	2004-197492	20040705
			US	2004-889657	20040712

GΙ

$$R^{3}$$
  $NR^{1}R^{2}$   $NR^{1}R^{2}$   $NR^{1}R^{2}$   $NR^{1}R^{2}$   $NR^{1}R^{2}$   $NR^{1}R^{2}$ 

Amino alc. derivs. or phosphonic acid derivs., pharmacol. acceptable salts AΒ thereof or pharmacol. acceptable esters thereof (I) [R1, R2 = H, lower alkyl, an amino-protecting group; R3 = H, lower alkyl, a hydroxy-protecting group; R4 = lower alkyl; n = an integer of 1 to 6; X = 0, (un)substituted; Y = ethylene,vinylene, ethynylene, COCH2, CH(OH)CH2, (un)substituted C6-10 arylene; Z = a single bond, C1-10 (un) substituted alkylene optionally containing O or S in or at terminus of the carbon chain; R5 = H, each (un)substituted C3-10cycloalkyl, C6-10 aryl, 5- o 7-membered heterocyclyl containing 1-3 of S, O, and/or N; R6, R7 = H, halo, lower alkyl, lower haloalkyl, lower alkoxy, lower alkylthio, CO2H, lower alkoxycarbonyl, HO, lower aliphatic acyl, NH2, mono- or di(lower alkyl) amino, lower aliphatic acylamino, cyano, NO2; provided that when R5 is hydrogen, then Z is branched or substituted C1-10 alkylene or C1-10 alkylene containing O or S in or at terminus of the carbon chain] are prepared These compds. possess an excellent immunosuppressive activity and are useful for the prevention or treatment of autoimmune diseases, chronic articular rheumatism, or organ transplant rejection. They are also used in combination with another immunosuppressant selected from (1) drugs inhibiting cellular signal related to cytokine expression of T cell, (2) drugs inhibiting nucleoside synthesis in immune cells, (3) drugs inhibiting the effect of cytokines against immune cells and possessing antirheumatic effect, (4) alkylating agents causing cell death by destruction of DNA chain or synthesis disorder of DNA, (5) antimetabolites inhibiting the nucleic acid metabolism by inhibiting the folic acid production, (6) protein prepns. possessing  $ext{TNF}lpha$ inhibitory activity, (7) steroid hormones forming complexes by binding to cellular steroid receptors and exhibiting an immunosuppressive activity through proteins synthesized by binding to the reactive site of chromosome, (8) substances inhibiting the production of prostaglandins, and /or (9) nonsteroidal antiinflammatory agents antagonizing prostaglandins. Thus, 4.23 q (2R)-1-acetoxy-2-acetylamino-2- methyl-4-(1-methylpyrrol-2-yl)butane was dissolved in 100 mL toluene, treated with a solution of 9.41 g 4-4dimethylaminopyridine and 7.92 g 5-phenylvaleryl chloride in 50 mL toluene, and stirred at 110° for 48 h to give 4.03 g (2R)-1-acetoxy-2-acetylamino-2methyl-4-[1-methyl-5-[5- phenyl-1-(5-phenylpentanoyloxy)pent-1-enyl]pyrrol-2yl]butane (45% yield) which (4.027 g) was dissolved in a mixture of 14 mL THF and 14 mL MeOH, treated with 14 mL H2O and 2.88 g LiOH.H2O, and stirred at  $50^{\circ}$ for 4 h to give, after workup, (2R)-2-amino-2-methyl-4-[1-methyl-5-(5-amino-2-methyl-4-[1-methylphenylpentanoyl)pyrrol-2-yl]butan-1-ol (II). II.HCl inhibited host vs. graft reaction of WKAH/Hkm or Lewis rat spleen cells transplanted s.c. in Lewis rat

rear soles with ID50 of 0.013 mg/kg. A tablet formulation 2-amino-2-methyl-4-[5-(5-phenylpentanoyl)thiophen-2-yl]butan-1-ol maleate was described.

MSTR 1

```
G7 = 18-4 \ 19-6 \ / \ 30-4 \ 32-6 \ / \ 38-4 \ 40-6 \ / \ 43-4 \ 44-6 \ / \ 45-4 \ 46-6
{}_{1}^{6}8 \overline{\phantom{0}}_{1}^{6}1^{3} \ {}_{3}^{6}1^{4} \overline{\phantom{0}}_{3}^{6}1^{5} \overline{\phantom{0}}_{3}^{6}1^{6} \ {}_{3}^{6}1^{9} \overline{\phantom{0}}_{6}1^{5} \overline{\phantom{0}}_{4}^{6}1^{8} \ {}_{4}^{6}2^{0} \overline{\phantom{0}}_{4}^{6}1^{5} \ {}_{4}^{6}2^{1} \overline{\phantom{0}}_{4}^{6}2^{5}
```

25(0)-G11

$$G13 = 35-18 \ 37-6 \ / \ 41-18 \ 42-6$$

 $_{3}$ §17—G15 $_{\overline{3}}$ §18  $_{4}$ 1616 $_{\overline{4}}$ 215

9<sup>6</sup>218—G15<del>9</del>618 9616<del>9</del>615

G39 = F

Patent location: claim 1
Note: or pharmacologically acceptable salts or esters
Note: additional heteroatom interruptions also claimed
Note: substitution is restricted

Note: Substitution is restricted also incorporates claim 4 and 7

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L89 ANSWER 13 OF 36 MARPAT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 139:133350 MARPAT  $\underline{\text{Full-text}}$ 

TITLE: Amidoacetonitrile derivatives useful as parasiticides,

and their preparation, compositions, and use

INVENTOR(S): Ducray, Pierre; Goebel, Thomas; Fruechtel, Joerg;

Bouvier, Jacques; Flum, Gabriela

PATENT ASSIGNEE(S): Novartis Ag, Switz.; Novartis Pharma Gmbh

SOURCE: PCT Int. Appl., 50 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA'	TENT I	.O		KIND DATE			APPLICATION NO.						DATE				
WO	2003	0598	68	 A:	1	2003	0724		W	D 20	 03-е:	 P498		2003	0120		
	W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
		CO,	CR,	CU,	CU, CZ, DE, DK,				DZ,	EC,	EE,	ES,	FΙ,	GB,	GD,	GE,	GH,
		HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KP,	KR,	KΖ,	LC,	LK,	LT,	LU,
		LV,	MA,	MD,	MK,	MN,	MX,	NO,	NZ,	OM,	PH,	PL,	PT,	RO,	RU,	SC,	SE,
		SG,	SK,	ΤJ,	TM,	TN,	TR,	TT,	UA,	US,	UZ,	VC,	VN,	YU,	ZA,	ZW	
	RW:	AM,	AZ,	BY,	KG,	KΖ,	MD,	RU,	ТJ,	TM,	AT,	BE,	ВG,	CH,	CY,	CZ,	DE,
		DK,	EE,	ES,	FΙ,	FR,	GB,	GR,	HU,	ΙE,	ΙT,	LU,	MC,	NL,	PT,	SE,	SI,
		SK,	TR														
	2468									A 20	03-2	4684	23	2003	0120		
AU				A1 20030730				A	U 20	03-2	0258	0	2003	0120			
EP	2 1470103			A.	1	2004	1027		E.	P 20	03-7	0153	1	2003	0120		
	R:					•								NL,	•		PT,
				LT, LV, FI, RO,											SK		
						20041103											
	16022																
	2005																
	5339	-											_	2003			
	20040																
	2005								U	S 20	04-5	0149	5	2004	0714		
	71538					2006											
	IN 2004CN01580										04-C						
	MX 2004PA07048					2004	1011				04-P.		8 20040721 20020121				
IORIT	Y APP	LN.	TNEO	.:													
									W	J 20	U3-E	P498		2003	0120		

104

$$Ar \xrightarrow{R^{1}} \begin{pmatrix} R^{2} & R^{3} & R^{5} \\ C_{N} & C_{N} & R^{4} \end{pmatrix} W \xrightarrow{R^{5}} \begin{pmatrix} R^{5} & R^{7} \\ C_{N} & R^{6} \end{pmatrix} M$$

$$(R^{8})_{n}$$

The invention relates to compds. I [in which R1 = H, alkyl, haloalkyl, AΒ cyanoalkyl, alkoxymethyl, or benzyl; R2, R3, R4, R5, R6 = H, halo, unsubstituted or mono- or polyhalogenated alk(en/yn)yl, (un)substituted alkoxy, haloalkoxy, cycloalkyl, or phenyl; or R2R3 = C2-6 alkylene; R7 = (un) substituted cycloalkoxy, cycloalkylthio, or [cycloalkyl] (R9) N, in which the substituents are halo, alkyl, hetaryl, or hetaryloxy; R8 = halo, NO2, cyano, (halo)alk(en)yl, (halo)alkoxy, alkynyl, cycloalkyl, alkenyloxy, haloalkenyloxy, alkylthio, haloalkylthio, alkylsulfonyloxy, haloalkylsulfonyloxy, alkylsulfinyl, haloalkylsulfinyl, alkylsulfonyl, haloalkylsulfonyl, alkenylthio, haloalkenylthio, (un)substituted Ph, PhO, PhNH, PhCO, PhCH(OH), etc.; or R7R8 = C3-5 alkylene; Ar = (un)substituted Ph, hetaryl, naphthyl, or quinolyl (substituents as given for R7, R8); R9 = H, alkyl, haloalkyl, allyl, alkoxymethyl, or COR10; R10 = alkyl, haloalkyl, or alkoxymethyl; W = 0, S, SO2, or N(R11); R11 = H or alkyl; p = 1, 2, 3, or 4; q = 0, 1, 2, 3, or 4; and n = 0-2; in which, if R7 = hetaryloxy, the hetaryl group in R7 is other than pyridyl; including enantiomers]. Compds. I have advantageous pesticidal properties, and are particularly suitable for controlling parasites in warm-blooded animals. A list of 120 possible specific compds. I is given, and one of these (II) is prepared and claimed per se. Claims include pharmaceutical and agrochem. compns., as well as use of I to control parasites. Thus, II was prepared in 6 steps: (1) Pd-catalyzed amination of 2-bromo-4,5-difluoroanisole with cyclopropylamine; (2) Nmethylation of the secondary amine product using NaH and MeI in DMF; (3) demethylation of the anisole methoxy group using BBr3; (4) etherification of the resultant phenol with chloroacetone using K2CO3 and KI; (5) aminocyanation of the ketone with NaCN and NH4Cl in aqueous NH3; and (6) amidation of the amino group with 4-(CF30)C6H4COCl and DMAP in CH2Cl2. II was active against the nematodes Trichostrongylus colubriformis and Haemonchus contortus in Mongolian gerbils, by peroral administration at doses in the range of 0.01 to 100 mg/kg. Tests for action against various ecto- and endo-parasitic insects and acarids, namely Lucilia sericata, Boophilus microplus, Amblyomma hebraeum, Dermanyssus gallinae, and Musca domestica, are described. Preferred formulations include granules, tablets, boluses, injectables, and pour-ons.

MSTR 1

G3 = 14-3 17-5

G7 = alkylene <containing 1-4 C, unbranched> (opt. substd. by 1 or more G20) G8 = 0 = alkylene <containing 1-4 C> G9 (opt. substd. by 1 or more G20) G13 G20 = F / carbon chain <containing 1 or more C, 0 or more double bonds, 0 or more triple bonds> (opt. substd. by 1 or more G4) alkoxy <containing 1 or more C> (opt. substd. by 1 or more G4) / Ph (opt. substd.) = Ph (opt. substd. by 1 or more G13) Patent location: claim 1 Note: also incorporates claim 8

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L89 ANSWER 14 OF 36 MARPAT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 138:304067 MARPAT Full-text

TITLE: Preparation of 1-cyano-1-methyl-2-phenoxyethyl

benzoates and phenylcarbamates for controlling parasites on warm-blooded animals

INVENTOR(S): Goebel, Thomas; Ducray, Pierre

PATENT ASSIGNEE(S): Novartis AG, Switz.; Novartis Pharma G.m.b.H.

SOURCE: PCT Int. Appl., 71 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PAI	PATENT NO. KIND			ИD	DATE APPLICATION NO.							Ο.	DATE					
									_									
WO	2003				2	2003	0417		W	0 20	02-E	P110	87	2002	1002			
WO	2003031393 A3				3	2003	1016											
	W: AE, AG,			AL,	AM,	AT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,	
		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	
		HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	KP,	KR,	KΖ,	LC,	LK,	LT,	LU,	
		LV,	MA,	MD,	MK,	MN,	MX,	NO,	NZ,	OM,	PH,	PL,	PT,	RO,	RU,	SE,	SG,	
		SI,	SK,	TJ.	TM.	TN.	TR,	TT,	UA,	US,	UZ,	VC,	VN.	YU,	ZA,	zw		

RW: AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR CA 2455999 A1 20030417 CA 2002-2455999 20021002 AU 2002349321 20030422 AU 2002-349321 20021002 Α1 EP 1434760 Α2 20040707 EP 2002-781206 20021002 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK BR 2002013125 A 20040921 BR 2002-13125 20021002 CN 1545500 Α 20041110 CN 2002-816448 20021002 JP 2005531489 20051020 JP 2003-534377 Τ 20021002 NZ 531640 NZ 2002-531640 20061130 20021002 Α RU 2296747 C2 RU 2004-114242 20070410 20021002 ZA 2004000562 20050407 ZA 2004-562 20040126 Α US 20040236137 20041125 US 2004-487167 20040217 Α1 B2 20070828 US 7262209 MX 2004PA03158 Α 20040727 MX 2004-PA3158 20040402 IN 2004CN00683 20060113 IN 2004-CN683 20040402 Α PRIORITY APPLN. INFO.: CH 2001-1829 20011004 WO 2002-EP11087 20021002

GΙ

$$Ar1 - X \longrightarrow O \xrightarrow{R^4 R^5} W \xrightarrow{R^7} Ar^2$$

$$\begin{array}{c}
 & \text{Me} \\
 & \text{Cl} \\
 & \text{CF3} \\
 & \text{II}
\end{array}$$

The title compds. [I; Ar1, Ar2 = (un)substituted Ph, NHPh, COPh, etc.; R4-R8 = H, halo, alkyl, etc.; W = O, S, SO2, NR9 (wherein R9 = H, alkyl); X = O, S, NR10 (R10 = H, alkyl, haloalkyl, allyl, alkoxymethyl); a = 1-4; b = 0-4] which are especially suitable for controlling parasites on warm-blooded animals, were prepared Thus, reacting 3-(2-chlorophenoxy)-2-hydroxy-2-methylpropionitrile (preparation given) with 4-trifluoromethylphenyl isocyanate in the presence of Et3N in CH2Cl2 afforded the title compound II.

MSTR 1

```
G9
     = (1) CN / Ph (opt. substd. by 1 or more G11)
G11
G12 = 35-6 \ 36-8
3514<del>3</del>615
```

G14 = 0

G15 = carbon chain < containing 1 or more C,

0 or more double bonds, 0 or more triple bonds>

(opt. substd. by 1 or more G16)

= F / Ph (opt. substd. by 1 or more G11) G16

Patent location: claim 1

substitution is restricted Note:

additional ring formation also claimed Note:

L89 ANSWER 15 OF 36 MARPAT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 138:304061 MARPAT Full-text

Preparation of cyanoacetamides for controlling TITLE:

parasites on warm-blooded animals
Ducray, Pierre; Goebel, Thomas
Novartis AG, Switz.; Novartis-Erfindungen

INVENTOR(S):

PATENT ASSIGNEE(S):

Verwaltungsgesellschaft m.b.H.

SOURCE: PCT Int. Appl., 59 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

```
PATENT NO. KIND DATE APPLICATION NO. DATE
                                                             _____
       WO 2003031394 A1 20030417 WO 2002-EP11088 20021002
             W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
                  CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
                   HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LT, LU,
                   LV, MA, MD, MK, MN, MX, NO, NZ, OM, PH, PL, PT, RO, RU, SE, SG,
                   SI, SK, TJ, TM, TN, TR, TT, UA, US, UZ, VC, VN, YU, ZA, ZW
             RW: AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE,
                   DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR
       CA 2458446 A1 20030417 CA 2002-2458446 20021002
AU 2002342791 A1 20030422 AU 2002-342791 20021002
EP 1436250 A1 20040714 EP 2002-779457 20021002
            R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
                  IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK
      BR 2002013066 A 20040928 BR 2002-13066 20021002
CN 1564809 A 20050112 CN 2002-819548 20021002
JP 2005504841 T 20050217 JP 2003-534378 20021002
NZ 531634 A 20051028 NZ 2002-531634 20021002
RU 2296119 C2 20070327 RU 2004-114240 20021002
ZA 2004001481 A 20050527 ZA 2004-1481 20040224
US 20040242913 A1 20041202 US 2004-489697 20040311
IN 2004CN00685 A 20060113 IN 2004-CN685 20040402
MX 2004PA03157 A 20060427 MX 2004-PA3157 20040402
RITY APPLN. INFO.:
CH 2001-1828 20021002
PRIORITY APPLN. INFO.:
                                                               WO 2002-EP11088 20021002
```

$$\begin{array}{c|c}
R9 & & & R4 & R5 & R7 \\
R10 & & & & & R6 & R8 \\
\end{array}$$

The title compds. [I; Ar1, Ar2 = (un) substituted Ph, NHPH, COPh, etc.; R4-R10, R12 = H, halo, alkyl, etc.; W = O, SOn, NR11 (wherein n = 0-2; R11 = H, alkyl); X = O, S, NR12; a = 1-4; b, c = 0-4] such as II which have advantageous pesticidal properties, were prepared One preparation example is given but no phys. data for intermediates and final product. Table of 783 compds. I is presented (data for only five of them are given).

MSTR 1

G21 = 0

4522<del>4</del>621

Patent location: claim 1

Note: substitution is restricted

Note: additional ring formation also claimed

INVENTOR(S):

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L89 ANSWER 16 OF 36 MARPAT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 137:124992 MARPAT Full-text

TITLE: Preparation of (acylamino)salicylic acids and their

use as agrochemical fungicides Hara, Yoshihiko; Saika, Michiyuki

PATENT ASSIGNEE(S): Nippon Soda Co., Ltd., Japan SOURCE: Jpn. Kokai Tokkyo Koho, 32 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002212157	A	20020731	JP 2001-89139	20010327
PRIORITY APPLN. INFO.	:		JP 2000-90870	20000329
			JP 2000-350481	20001117

GΙ

AB Title compds. I [R1 = H, C1-4 alkyl; A = (un)substituted C1-6 alkylene; X = 0, NR3, CR3R4; R2 = (un)substituted C1-16 alkyl, (un)substituted C3-10 cycloalkyl, (un)substituted C2-10 alkenyl, etc.; R3, R4 = H, C1-10 alkyl, C2-6 alkenyl, C2-6 alkynyl, C1-6 alkoxy; NR2R3 may form ring] and their salts are prepared Thus, N-(1-n-heptyloxycarbonylethyl)-2-benzyloxy-3- nitrobenzamide was hydrogenated over Pd/C in AcOEt, filtered, evaporated, and treated with N-formylimidazole in CH2C12 to give 53% I (R1 = H, A = CHMe, XR2 = OC7H15-n), which showed ≥75% antifungal activity against Venturia inaequalis.

MSTR 1

G2 = alkylene <containing 1 or more C> (opt. substd. by 1 or more G3)

G3 = alkenyl <containing 2-8 C> (opt. substd. by 1 or more G4)

```
alkynyl <containing 2-8 C> (opt. substd. by 1 or more G4) /
          Ph (opt. substd. by 1 or more G7) / OH /
          alkoxycarbonyl <containing 1-8 C> /
          alkylaminocarbonyl <containing 1-8 C>
G7
        = F
G12
       = 28
 28(0)—G23
G14 = alkenyl <containing 2-10 C>
         (opt. substd. by 1 or more G16)
     = Ph (opt. substd. by 1 or more G7) / F
G18
     = 0
G23
     = 29
 2618—G14
Patent location: claim 1
Note:
                               or salts
L89 ANSWER 17 OF 36 MARPAT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 131:165311 MARPAT Full-text
                            New carboxylic acid derivatives with 5-substituted
TITLE:
                           pyrimidine ring, their preparation and use as
                            endothelin receptor antagonists
                            Amberg, Wilhelm; Jansen, Rolf; Kling, Andreas; Klinge,
INVENTOR(S):
                            Dagmar; Riechers, Hartmut; Hergenroeder, Stefan;
                            Raschack, Manfred; Unger, Liliane
                          BASF A.-G., Germany
PATENT ASSIGNEE(S):
                            Ger. Offen., 20 pp.
SOURCE:
                            CODEN: GWXXBX
DOCUMENT TYPE:
                           Patent
LANGUAGE:
                            German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:
     PATENT NO. KIND DATE APPLICATION NO. DATE
     DE 19806438 A1 19990819 DE 1998-19806438 19980217
CA 2321182 A1 19990826 CA 1999-2321182 19990205
WO 9942453 A1 19990826 WO 1999-EP776 19990205
          W: AL, AU, BG, BR, BY, CA, CN, CZ, GE, HR, HU, ID, IL, IN, JP, KR,
              KZ, LT, LV, MK, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, UA, US,
              AM, AZ, KG, MD, TJ, TM
          RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
              PT, SE
     AU 9930271
BR 9907911
                        A 19990906 AU 1999-30271 19990205

      BR 9907911
      A
      20001024
      BR 1999-7911
      19990205

      TR 200002376
      T2
      20001221
      TR 2000-2376
      19990205

      EP 1066268
      A1
      20010110
      EP 1999-911657
      19990205

          R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE,
              SI, FI, RO
```

JP 2002503726 T 20020205 JP 2000-532405 19990205

HU	2001000957	A2	20020228	HU	2001-957	19990205
TW	579376	В	20040311	TW	1999-88102031	19990210
ZA	9901214	A	20000816	ZA	1999-1214	19990216
MX	2000PA06463	A	20010219	MX	2000-PA6463	20000629
BG	104577	A	20010330	ВG	2000-104577	20000704
IN	2000CN00227	A	20050304	IN	2000-CN227	20000728
NO	2000004075	A	20000815	NO	2000-4075	20000815
HR	2000000602	A1	20010630	HR	2000-602	20000913
PRIORIT	Y APPLN. INFO.:			DE	1998-19806438	19980217
				WO	1999-EP776	19990205

GΙ

$$R^{6}ZCR^{4}R^{5}CHR^{1}O$$
 $N$ 
 $R^{2}$ 
 $R^{3}$ 

The title compds. [I; R1 = tetrazolyl, C(O)R; R = OR7, (substituted) N-linked AΒ 5-membered heteroarom. residue, O(CH2)pS(:0)kR8, NHSO2R9; R7 = H, cation, (substituted) C3-8 cycloalkyl, (substituted) C1-8 alkyl, (substituted) Ph, (substituted) CH2Ph, C3-6 (halo)alkenyl, C3-6 (halo)alkynyl; R8, R9 = (substituted) C1-4 alkyl, (substituted) C3-8 cycloalkyl, (substituted) C3-6 alkenyl, (substituted) C3-6 alkynyl, (substituted) Ph; k = 0-2; p = 1-4; R2, R3 = H, OH, (substituted) amino, halo, alkyl, alkenyl, alkynyl, hydroxyalkyl, haloalkyl, alkoxy, etc.; R4, R5 = (substituted) Ph, (substituted) naphthyl, C3-7 cycloalkyl, etc.; R6 = H, (substituted) C1-8 alkyl, (substituted) C3-6 alkenyl, (substituted) C3-6 alkynyl, (substituted) C3-8 cycloalkyl, (substituted) Ph, (substituted) naphthyl, (substituted) 5- or 6-membered heteroarom. residue; X = halo, C1-4 haloalkyl, OH; Z = O, S, single bond],their enantiomers, diastereomers, and physiol. compatible salts are useful as endothelin receptor antagonists for treatment of diseases associated with elevated endothelin levels, such as chronic cardiac insufficiency, restenosis, hypertension, acute or chronic kidney failure, cerebral ischemia, asthma, benign prostate hyperplasia, and prostate cancer. Thus, Me 2-hydroxy-3methoxy-3,3-diphenylpropionate reacted with NaH and 4,6-dimethoxy-5-fluoro-2methylsulfonylpyrimidine in DMF to produce I (R1 = CO2Me, R2 = R3 = OMe, R4 = R5 = Ph, R6 = Me, X = F, Z = O), which was saponified to the corresponding acid (R1 = CO2H) (II). II bound to endothelin ETA and ETB receptors with Ki 7.4 and 1200 nM, resp.

MSTR 1A

$$G27 - G35 - G25$$
 $G25 - G1 - G23$ 
 $G23$ 

G1 = tetrazolyl

G25 = Ph (opt. substd. by 1 or more G26)

G26 = F

G27 = alkenyl < containing 3-6 C >

(opt. substd. by 1 or more G28)

G28 = F / Ph (opt. substd. by (1-3) G29)

G35 = 0

Derivative: and physiologically acceptable salts

Patent location: claim 1

Note: substitution is restricted

Note: additional ring formation also claimed Stereochemistry: and enantiomeric and diastereomeric forms

L89 ANSWER 18 OF 36 MARPAT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 130:257367 MARPAT Full-text

TITLE: Multicomponent pharmaceutical formulations for

treatment of vasoconstrictive disorders Kirchengast, Michael; Muenter, Klaus

INVENTOR(S): Kirchengast, Michael; Muenter, Klaus PATENT ASSIGNEE(S): Knoll A.-G. Chemische Fabriken, Germany

SOURCE: Ger. Offen., 34 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

DE 19743143 A1 19990401 DE 1997-19743143 19970930 CA 2304698 A1 19990408 CA 1998-2304698 19980910 CA 2304698 C 20080219	
CA 2304698 A1 19990408 CA 1998-2304698 19980910 CA 2304698 C 20080219	
CA 2304698 C 20080219	
WO 9916444 A1 19990408 WO 1998-EP5772 19980910	
W: AL, AU, BG, BR, BY, CA, CN, CZ, GE, HU, ID, IL, JP, KR, KZ,	
LV, MK, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, UA, US, AM,	·
KG, MD, TJ, TM	
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC,	NL,
PT, SE	
AU 9892672 A 19990423 AU 1998-92672 19980910	
AU 739860 B2 20011025	
EP 1019055 A1 20000719 EP 1998-945323 19980910	
EP 1019055 B1 20030507	
R: AT, BE, CH, DE, ES, FR, GB, IT, LI, NL, SE, FI	
BR 9812404 A 20000919 BR 1998-12404 19980910	
JP 2001517703 T 20011009 JP 2000-513580 19980910	
HU 2000004590 A2 20011128 HU 2000-4590 19980910	
AT 239479 T 20030515 AT 1998-945323 19980910	
AT 239479 T 20030515 AT 1998-945323 19980910 RU 2213577 C2 20031010 RU 2000-111500 19980910 ES 2199461 T3 20040216 ES 1998-945323 19980910	
ES 2199461 T3 20040216 ES 1998-945323 19980910	
CZ 298745 B6 20080116 CZ 2000-1081 19980910	
MX 200002654 A 20001211 MX 2000-2654 20000316	
US 6352992 B1 20020305 US 2000-508989 20000320	
NO 2000001634 A 20000329 NO 2000-1634 20000329	
NO 319048 B1 20050606	
HK 1032355 A1 20050304 HK 2001-102973 20010425	
PRIORITY APPLN. INFO.: DE 1997-19743143 19970930	
WO 1998-EP5772 19980910	

GΙ

Novel combinations of an endothelin antagonist and a  $\beta$ -receptor blocker are provided for treatment of vasoconstrictive disorders. The endothelin antagonist is a pyrimidine- or triazine-substituted carboxylic acid [I; R = CHO, CN, CO2H, tetrazolyl, etc.; R2, R3 = H, OH, amino, halo, C1-4 alkyl, haloalkyl, alkoxy, etc.; R4, R5 = (substituted) Ph or naphthyl, C3-7 cycloalkyl; R6 = H, (substituted) alkyl, alkenyl, alkynyl, or cycloalkyl; X = N, CR14; R14 = H, C1-5 alkyl; or R14CCR3 = 5- or 6-membered ring; Y = O, S, single bond; Z = O, S, SO, SO2, single bond] or related compound Thus, hard gelatin capsules were filled with I (R = CO2H, R2 = R3 = OMe, R4 = R5 = Ph, R6 = Me, X = CH, Y = Z = O) 100.0, bucindolol 30.0, lactose 18.0, PVP 15.0, microcryst. cellulose 17.5, Na carboxymethylstarch 10.0, talc 9.0, and Mg stearate 3.0 mg.

MSTR 1

G 2 7—G 3

G1 = tetrazolyl

G3 = 64

6 G 2 4—G 2 5

G13 = Ph (opt. substd. by 1 or more G14)

G14 = halo

G17 = alkenyl <containing 3-6 C>

(opt. substd. by 1 or more G18)

G18 = halo / Ph (opt. substd.)

G23 = 0

G24 = 0

G27 = 4

Patent location:

claim 1

Note: additional ring formation also claimed

MSTR 5

$$G17-G23-G13$$
 $G17-G23-G1$ 
 $G13-G1$ 
 $G12-G3$ 
 $G5$ 
 $G5$ 

G1 = tetrazolyl

G13 = Ph (opt. substd. by 1 or more G14)

G14 = halo

G17 = alkenyl < containing 3-6 C>

(opt. substd. by 1 or more G18)

G18 = halo / Ph (opt. substd.)

G23 = 0

Patent location: claim 1

Note: additional ring formation also claimed

L89 ANSWER 19 OF 36 MARPAT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 130:257366 MARPAT Full-text

TITLE: Multicomponent pharmaceutical formulations for

treatment of cardiovascular disorders

INVENTOR(S): Muenter, Klaus; Kirchengast, Michael; Hergenroeder,

Stefan

PATENT ASSIGNEE(S): Knoll A.-G. Chemische Fabriken, Germany

SOURCE: Ger. Offen., 34 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA'	TENT	NO.		KII	ND 	DATE			A:	PPLI	CATI	ON NC	). 	DATE			
	1974													1997			
WO	9916	446		А	Τ	1999	0408		M (	0 19	98-E.	P291	C	1998	091/		
	W:	AL,	ΑU,	BG,	BR,	BY,	CA,	CN,	CZ,	GE,	HU,	ID,	IL,	JP,	KR,	KΖ,	LT,
		LV,	MK,	MX,	NO,	NZ,	PL,	RO,	RU,	SG,	SI,	SK,	TR,	UA,	US,	AM,	ΑZ,
		BY,	KG,	KΖ,	MD,	RU,	ТJ,	TM									
	RW:	AT,	BE,	CH,	CY,	DE,	DK,	ES,	FI,	FR,	GB,	GR,	IE,	ΙΤ,	LU,	MC,	NL,
		PT,	SE														
AU	9897	447		А		1999	0423		A	U 19	98-9	7447		1998	0917		
PRIORIT	Y APP	LN.	INFO	.:					D:	E 19	97-1	9743	142	1997	0930		
									M	0 19	98-E	P591	5	1998	0917		

GΙ

Novel combinations of an endothelin antagonist and a calcium antagonist are provided for treatment of cardiovascular disorders. The endothelin antagonist is a pyrimidine- or triazine-substituted carboxylic acid [I; R = CHO, CN, CO2H, tetrazolyl, etc.; R2, R3 = H, OH, amino, halo, C1-4 alkyl, haloalkyl, alkoxy, etc.; R4, R5 = (substituted) Ph or naphthyl, C3-7 cycloalkyl; R6 = H, (substituted) alkyl, alkenyl, alkynyl, or cycloalkyl; X = N, CR14; R14 = H, C1-5 alkyl; or R14CCR3 = 5- or 6-membered ring; Y = O, S, single bond; Z = O, S, SO, SO2, single bond] or related compound Thus, hard gelatin capsules were filled with I (R = CO2H, R2 = R3 = OMe, R4 = R5 = Ph, R6 = Me, X = CH, Y = Z = O) 100.0, gallopamil 75.0, lactose 18.0, PVP 15.0, microcryst. cellulose 17.5, Na carboxymethylstarch 10.0, talc 9.0, and Mg stearate 3.0 mg.

MSTR 1

G 2 7—G 3

G1 = tetrazolyl

G3 = 64

6 4 2 4—G 2 5

G13 = Ph (opt. substd. by 1 or more G14)

G14 = halo

G17 = alkenyl <containing 3-6 C>

(opt. substd. by 1 or more G18)

G18 = halo / Ph (opt. substd.)

G23 = 0

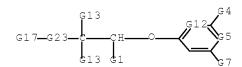
G24 = 0

G27 = 4

Patent location: claim

Note: additional ring formation also claimed

MSTR 5



G1 = tetrazolyl

G13 = Ph (opt. substd. by 1 or more G14)

G14 = halo

G17 = alkenyl <containing 3-6 C>

(opt. substd. by 1 or more G18)

G18 = halo / Ph (opt. substd.)

G23 = 0

Patent location: claim 1

Note: additional ring formation also claimed

L89 ANSWER 20 OF 36 MARPAT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 130:257365 MARPAT Full-text

TITLE: Multicomponent pharmaceutical formulations for

treatment of kidney failure

INVENTOR(S): Hahn, Alfred; Kirchengast, Michael; Muenter, Klaus

PATENT ASSIGNEE(S): Knoll A.-G. Chemische Fabriken, Germany

SOURCE: Ger. Offen., 34 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PA.	TENT	NO.		KI	ND	DATE			Al	PPLI	CATI	ON NO	٥.	DATE			
	1974																
	2304																
WO	9916	445		A	1	1999	0408		M	0 19	98-E	P5773	3	1998	0910		
	W:	AL,	ΑU,	ВG,	BR,	BY,	CA,	CN,	CZ,	GE,	HU,	ID,	IL,	JP,	KR,	KΖ,	LT,
		LV,	MK,	MX,	NO,	NΖ,	PL,	RO,	RU,	SG,	SI,	SK,	TR,	UA,	US,	ΑM,	ΑZ,
		KG,	MD,	ΤJ,	TM												
	RW:	AT, PT,	•	CH,	CY,	DE,	DK,	ES,	FI,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,
AU	9895	395		А		1999	0423		Αl	U 19	98-9	5395		1998	0910		
	7507																
	1014								E	P 19	98-9	48954	4	1998	0910		
	1014																
									IT,	LI,	NL,	SE,	FΙ				
JP	2001													1998	0910		
	2000																
AT	2577	06		Τ		2004	0115		A'	Т 19	98-9	48954	4	1998	0910		
ES	2214	734		Τ	3	2004	0916		E	S 19	98-9	48954	4	1998	0910		
	6329																
	2000													2000			
	3243																
RIORIT									D)	E 19	97-1	9742	717	1997	0926		
									D	E 19	97-1	97431	141	1997	0930		
									M	0 19	98-E	P5773	3	1998	0910		

GΙ

AB Novel combinations of an endothelin antagonist and an ACE inhibitor are provided for treatment of kidney failure. The endothelin antagonist is a pyrimidine- or triazine-substituted carboxylic acid [I; R = CHO, CN, CO2H, tetrazolyl, etc.; R2, R3 = H, OH, amino, halo, C1-4 alkyl, haloalkyl, alkoxy, etc.; R4, R5 = (substituted) Ph or naphthyl, C3-7 cycloalkyl; R6 = H, (substituted) alkyl, alkenyl, alkynyl, or cycloalkyl; X = N, CR14; R14 = H, C1-5 alkyl; or R14CCR3 = 5- or 6-membered ring; Y = O, S, single bond; Z = O, S, SO, SO2, single bond] or related compound Thus, hard gelatin capsules were filled with I (R = CO2H, R2 = R3 = OMe, R4 = R5 = Ph, R6 = Me, X = CH, Y = Z = O) 100.0, ramipril 2.5, lactose 18.0, PVP 15.0, microcryst. cellulose 17.5, Na carboxymethylstarch 10.0, talc 9.0, and Mg stearate 3.0 mg.

MSTR 1

G 2 7—G 3

G1 = tetrazolyl

G3 = 64

6<sup>4</sup>24<del>-</del>625

G13 = Ph (opt. substd. by 1 or more G14)

G14 = halo

G17 = alkenyl < containing 3-6 C>

(opt. substd. by 1 or more G18)

G18 = halo / Ph (opt. substd.)

G23 = 0

G24 = 0

G27 = 4

Patent location:

claim 1

Note: additional ring formation also claimed

MSTR 5

G1 = tetrazolyl

G13 = Ph (opt. substd. by 1 or more G14)

G14 = halo

G17 = alkenyl <containing 3-6 C>

(opt. substd. by 1 or more G18)

G18 = halo / Ph (opt. substd.)

G23 = 0

Patent location: claim 1

Note: additional ring formation also claimed

L89 ANSWER 21 OF 36 MARPAT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 130:257364 MARPAT Full-text

TITLE: Multicomponent pharmaceutical formulations for

treatment of cardiovascular disorders

INVENTOR(S): Muenter, Klaus; Kirchengast, Michael; Klein, Gisela;

Korioth, Horst

PATENT ASSIGNEE(S): Knoll A.-G. Chemische Fabriken, Germany

SOURCE: Ger. Offen., 34 pp.

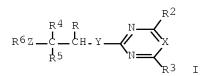
CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19743140	A1	19990401	DE 1997-19743140	19970930
PRIORITY APPLN. INFO.	:		DE 1997-19743140	19970930
GI				



AB Novel combinations of an endothelin antagonist and a vasodilator are provided for treatment of cardiovascular disorders. The endothelin antagonist is a pyrimidine- or triazine-substituted carboxylic acid [I; R = CHO, CN, CO2H,

tetrazolyl, etc.; R2, R3 = H, OH, amino, halo, C1-4 alkyl, haloalkyl, alkoxy, etc.; R4, R5 = (substituted) Ph or naphthyl, C3-7 cycloalkyl; R6 = H, (substituted) alkyl, alkenyl, alkynyl, or cycloalkyl; X = N, CR14; R14 = H, C1-5 alkyl; or R14CCR3 = 5- or 6-membered ring; Y = O, S, single bond; Z = O, S, S0, S02, single bond] or related compound Thus, administration of a combination of I (R = C02H, R2 = R3 = OMe, R4 = R5 = Ph, R6 = Me, X = CH, Y = Z = O) (II) and hydralazine (5 and 0.5 mg/kg, resp.) orally to normal male beagles synergistically decreased their mean arterial pressure after 2 h by 15.4 mm Hg. Hard gelatin capsules were prepared containing II 200.0, hydralazine 50.0, lactose 18.0, PVP 15.0, microcryst. cellulose 17.5, Na carboxymethylstarch 10.0, talc 9.0, and Mg stearate 3.0 mg.

MSTR 1

G 2 7\_G 3

G1 = tetrazolyl

G3 = 64

6924-G25

G13 = Ph (opt. substd. by 1 or more G14)

G14 = halo

G17 = alkenyl < containing 3-6 C>

(opt. substd. by 1 or more G18)

G18 = halo / Ph (opt. substd.)

G23 = 0

G24 = O

G27 = 4

Patent location: claim 1

Note: additional ring formation also claimed

MSTR 5

```
= tetrazolyl
        = Ph (opt. substd. by 1 or more G14)
G14
        = halo
     = alkenyl <containing 3-6 C>
G17
          (opt. substd. by 1 or more G18)
     = halo / Ph (opt. substd.)
G18
     = 0
Patent location:
Note:
                                   additional ring formation also claimed
L89 ANSWER 22 OF 36 MARPAT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 130:257363 MARPAT Full-text
TITLE:
                              Multicomponent pharmaceutical formulations for
                              treatment of cardiovascular disorders
INVENTOR(S):
                              Muenter, Klaus; Kirchengast, Michael; Korioth, Horst
                          Knoll A.-G. Chemische Fabriken, Germany
PATENT ASSIGNEE(S):
                               Ger. Offen., 36 pp.
SOURCE:
                               CODEN: GWXXBX
DOCUMENT TYPE:
                              Patent
LANGUAGE:
                               German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:
      DE 19742717

KIND DATE APPLICATION NO. DATE
      DE 19742717 A1 19990401 DE 1997-19742717 19970926 CA 2304712 A1 19990408 CA 1998-2304712 19980910 WO 9916445 A1 19990408 WO 1998-EP5773 19980910
           W: AL, AU, BG, BR, BY, CA, CN, CZ, GE, HU, ID, IL, JP, KR, KZ, LT,
                LV, MK, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, UA, US, AM, AZ,
                KG, MD, TJ, TM
           RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
                PT, SE
      AU 9895395 A 19990423 AU 1998-95395 19980910
AU 750755 B2 20020725
EP 1014989 A1 20000705 EP 1998-948954 19980910
EP 1014989 B1 20040114
           R: AT, BE, CH, DE, ES, FR, GB, IT, LI, NL, SE, FI
     HU 2000004298 A2 20011128 HU 2000-4298 19980910
AT 257706 T 20040115 AT 1998-948954 19980910
RU 2222328 C2 20040127 RU 2000-110630 19980910
ES 2214734 T3 20040916 ES 1998-948954 19980910
MX 200002655 A 20001211 MX 2000-2655 20000316
US 6329384 B1 20011211 US 2000-508993 20000320
NO 2000001548 A 20000324 NO 2000-1548 20000324
NO 324382 B1 20071001
RITY APPLN. INFO.:
      JP 2001517704 T 20011009 JP 2000-513581 19980910
PRIORITY APPLN. INFO.:
                                                      DE 1997-19743141 19970930
                                                      WO 1998-EP5773 19980910
GΙ
```

121

$$R^{6}Z$$
  $\stackrel{R^{4}}{\underset{R}{\overset{R}{\overset{}}{\overset{}}{\overset{}}}}$   $\stackrel{R}{\underset{R^{3}}{\overset{}}}$   $\stackrel{R^{2}}{\underset{R^{3}}{\overset{}}}$ 

Novel combinations of an endothelin antagonist and an inhibitor of the renin-AΒ angiotensin system are provided for treatment of cardiovascular disorders. The endothelin antagonist is a pyrimidine- or triazine-substituted carboxylic acid [I; R = CHO, CN, CO2H, tetrazolyl, etc.; R2, R3 = H, OH, amino, halo, C1-4 alkyl, haloalkyl, alkoxy, etc.; R4, R5 = (substituted) Ph or naphthyl, C3-7 cycloalkyl; R6 = H, (substituted) alkyl, alkenyl, alkynyl, or cycloalkyl; X = N, CR14; R14 = H, C1-5 alkyl; or R14CCR3 = 5- or 6-membered ring; Y = 0, S, single bond; Z = O, S, SO, SO2, single bond] or related compound Thus, administration of a combination of I (R = CO2H, R2 = R3 = OMe, R4 = R5 = Ph, R6 = Me, X = CH, Y = Z = O) (II) and trandolapril (2 and 10 mg/kg, resp.) orally to normal male beagles decreased their mean arterial pressure after 2 h by 30.9 mm Hg and increased the heart rate by 25.4/min. Hard gelatin capsules were prepared containing II 250.0, ramipril 2.5, lactose 18.0, PVP 15.0, microcryst. cellulose 17.5, Na carboxymethylstarch 10.0, talc 9.0, and Mg stearate 3.0 mg.

MSTR 1

G 2 7**—**G 3

G1 = tetrazolyl

G3 = 64

6924—G25

G13 = Ph (opt. substd. by 1 or more G14)

G14 = halo

G17 = alkenyl <containing 3-6 C>

(opt. substd. by 1 or more G18)

G18 = halo / Ph (opt. substd.)

G23 = 0

G24 = 0

G27 = 4

Patent location: claim 1

Note: additional ring formation also claimed

MSTR 5

G1 = tetrazolyl

G13 = Ph (opt. substd. by 1 or more G14)

G14 = halo

G17 = alkenyl <containing 3-6 C>

(opt. substd. by 1 or more G18)

G18 = halo / Ph (opt. substd.)

G23 = 0

Patent location: claim 1

Note: additional ring formation also claimed

L89 ANSWER 23 OF 36 MARPAT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 129:275935 MARPAT Full-text

TITLE: Novel pyrimidine- and triazine-containing carboxylic

acid derivatives, their preparation, and use as endothelin receptor antagonists in treating cancer

INVENTOR(S): Romerdahl, Cynthia A.

PATENT ASSIGNEE(S): BASF A.-G., Germany
SOURCE: PCT Int. Appl., 100 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PAT	ΓΕΝΤ	NO.		KII	ND	DATE			Al	PPLI	CATI	N NC	٥.	DATE			
WO	9841	206		 A:	1	1998	0924		M	) 19	 98-U	S459	6	1998	0309		
	W:	AL,	AM,	ΑT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CU,	CZ,	DE,
		DK,	EE,	ES,	FI,	GB,	GE,	GH,	GM,	GW,	HU,	ID,	IL,	IS,	JP,	KE,	KG,
		ΚP,	KR,	KΖ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MD,	MG,	MK,	MN,	MW,	MX,
		NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ТJ,	TM,	TR,	TT,
		UA,	UG,	US,	UZ,	VN,	YU,	ZW									
	RW:	GH,	GM,	KE,	LS,	MW,	SD,	SZ,	UG,	ZW,	ΑT,	BE,	CH,	DE,	DK,	ES,	FI,
		FR,	GB,	GR,	IE,	ΙΤ,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	CM,
		GA,	GN,	ML,	MR,	NE,	SN,	TD,	TG								
US	6030	975		А		2000	0229		U	S 19	97-8	1862.	2	1997	0314		
CA	2283	732		A	1	1998	0924		C	A 19	98-2	2837.	32	1998	0309		
ΑU	9866	946		А		1998	1012		Αl	J 19	98-6	6946		1998	0309		
AU	7440	19		В	2	2002	0214										
EP	9698	41		A.	1	2000	0112		E	2 19	98-9	0906	7	1998	0309		
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙΤ,	LI,	LU,	NL,	SE,	PT,	IE,
		SI,	FI,	RO													
BR	9808	263		А		2000	0516		B	R 19	98-8	263		1998	0309		

HU 2000002	249 A2	20010528	HU	2000-2249	19980309
HU 2000002	249 A3	20011128			
JP 2001517	220 T	20011002	JP	1998-540573	19980309
IN 1998MA0	0509 A	20050304	IN	1998-MA509	19980312
ZA 9802136	A	19990913	ZA	1998-2136	19980313
NO 9904426	A	19991112	ИО	1999-4426	19990913
PRIORITY APPLN.	INFO.:		US	1997-818622	19970314
			WO	1998-US4596	19980309

GΙ

AΒ The invention provides a method for treating cancer, wherein the cancer is a tumor in which endothelin (ET) is upregulated (e.g. tumors of the prostate, lung, liver, breast, brain, stomach, colon, endometrium, testicle, thyroid, pituitary, bladder, kidney, pancreas and meninges), by administering a compound I [R = CHO, tetrazolyl, cyano, CO2H or its hydrolyzable derivs.; R2 = H, OH, (di)(alkyl)amino, halo, alkyl, haloalkyl, alkoxy, haloalkoxy, alkylthio; X = N, CH, C-alkyl, or forms a 5- or 6-ring to R3; R3 = groups given for R2, or NHO-alkyl, or forms 5- or 6-ring to X; R4, R5 = (un) substituted Ph, naphthyl, or certain fused derivs.; or R4 = a wide variety of possible substituents and R5 = H, alk(en/yn)yl, cycloalkyl, haloalkyl, Ph, etc.; or R4R5 forms (un)substituted 3- to 8-ring; R6 = H, (un)substituted alk(en/yn)yl, cycloalkyl, Ph, naphthyl, heteroaryl; Y, Z = S, O, bond; with provisos]. Over 150 compds. were prepared For instance, methanolysis of Me 3,3-diphenyl-2,3-epoxypropionate in the presence of BF3.OEt2 gave 88% Me 2hydroxy-3-methoxy-3,3-diphenylpropionate, which was etherified with 4,6dimethoxy-2-(methylsulfonyl)pyrimidine to give 82% title compound II. At 150 mg/kg/day i.p. in mice in the DU-145 prostate tumor model, II reduced mean tumor weight to 33% of control after 10 days.

MSTR 1B

```
G1 = tetrazolyl

G8 = Ph (opt. substd. by 1 or more G9)

G9 = halo

G15 = 235
```

2952-G23

G16 = halo / Ph (opt. substd.)

G22 = 0

G23 = alkenyl < containing 3-6 C >

(opt. substd. by 1 or more G16)

G24 = 0

Patent location: claim 1

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L89 ANSWER 24 OF 36 MARPAT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 127:358879 MARPAT Full-text

TITLE: Preparation of 1-(3-heterocyclylphenyl)-s-triazine-

2,4,6-oxo- or -thiotrione herbicidal agents Crews, Alvin Donald, Jr.; Karp, Gary Mitchell;

INVENTOR(S): Crews, Alvin Donald, Jr.; Karp, Gary Mitchell;

Manfredi, Mark Christopher; Guaciaro, Michael Anthony

PATENT ASSIGNEE(S): American Cyanamid Company, USA

SOURCE: U.S., 49 pp. CODEN: USXXAM

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

US 5679791 A 19971021 US 1996-686288 19960725

PRIORITY APPLN. INFO: US 1996-686288 19960725

OTHER SOURCE(S): CASREACT 127:358879

GΙ

### \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

The title compds. [I; R = H, C1-6 alkyl, C2-12 alkoxyalkyl, etc.; R1 = H, C3-6 alkenyl, C3-6 alkynyl, etc.; R11, R12 = H, (un)substituted C1-6 alkyl, C3-6 cycloalkyl; R11R12 = (un)substituted 4-7 membered (un)saturated ring optionally interrupted by O, S(O)r, or N; A, A1, A2 = O, S; r = 0-2; X, Y = H, halo, NO2, CN], useful for the control of undesirable plant species, were prepared by reacting an isothiocyanate II with a hydrazine R12NHNHR11 followed by reaction of the resulting intermediate III with phosgene or a phosgene equivalent in the presence of a base. Thus, the title compound IV showed 100% efficacy against, e.g., common lambsquarters in preemergence test at 0.125 kg/ha.

MSTR 1

G6 = alkyl <containing 1-12 C> (opt. substd. by 1 or more G7)
G7 = CN / 26 / 34 / OH / 45 / 48 / Ph (opt. substd. by (1-3) G21)

2C(0)-G8 H2C 0 C(0)-G19 H2C G18 G20 0 G2

G8 = 38

389---G10

G9 = 0

G10 = alkenyl <containing 3-6 C> (opt. substd. by 1 or more G13)

G13 = F / Ph (opt. substd. by 1 or more G12)

G21 = F

Patent location: claim 1

Note: substitution is restricted

MSTR 2

$$G8 = 38$$

G9 = O

G10 = alkenyl <containing 3-6 C>

(opt. substd. by 1 or more G13)

G13 = F / Ph (opt. substd. by 1 or more G12)

G21 = F

Patent location: claim 1

Note: substitution is restricted

MSTR 4

$$G6 = alkyl < containing 1-12 C >$$

(opt. substd. by 1 or more G7)

G7 = CN / 26 / 99 / 34 / OH / 45 / 48 / COLOR COLOR

Ph (opt. substd. by (1-3) G21)

$$_{2}$$
\$(0).G8  $_{9}$ \$\frac{\mathbb{G}}{\mathbb{G}} = \mathbb{G}\_{1}9 \quad \mathbb{H}\_{3}^{2}\$\mathbb{G}\_{4}\$\quad \mathbb{G}\_{1}9 \quad \mathbb{H}\_{4}^{2}\$\mathbb{G}\_{2}\$\quad \mathbb{G}\_{1}8\$

$$G8 = 38$$

389-G10

G9 = O

G10 = alkenyl <containing 3-6 C>

(opt. substd. by 1 or more G13)

G13 = F / Ph (opt. substd. by 1 or more G12)

G21 = F

Patent location: disclosure

Note: substitution is restricted

Note: additional ring formation also disclosed

L89 ANSWER 25 OF 36 MARPAT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 127:346409 MARPAT Full-text

TITLE: Preparation of pyrimidinyloxypropionates and related

compounds as endothelin antagonists.

INVENTOR(S): Amberg, Wilhelm; Kling, Andreas; Klinge, Dagmar;

Riechers, Hartmut; Baumann, Ernst; Unger, Liliane; Raschack, Manfred; Hergenroeder, Stefan; Schult,

Sabine

PATENT ASSIGNEE(S): BASF A.-G., Germany SOURCE: Ger. Offen., 25 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA:	rent	NO.		KI	ND	DATE			A.	PPLI	CATI	ON NO	ο.	DATE				
CA	225	 14542 0764 8982		А	1	1997	1023		C	A 19	97-2	2507	64	1997	0404			
	W:	AU, RO,	BG, RU,	BR, SG,	CA, SI,	CN, SK,	CZ, TR,	GE, UA,	HU, US,	IL, AM,	JP, AZ,	KR, BY,	LV, KG,	MX, KZ,	NO, MD,	TJ,	TM	SE
AU	RW: AT, AU 9726364 AU 711293 EP 892788 R: AT,																	
AU	711:	293		В	2	1999	1007											
EP	892	788		Α	1	1999	0127		E.	P 19	97-9	1810	9	1997	0404			
	R:	,	,	,	DE,	DK,	ES,	FR,	GB,	GR,	ΙΤ,	LI,	LU,	NL,	SE,	PT,	IE,	
			FΙ,															
NZ	331	704		А		2000	0623		N	Z 19	97-3	3170	4	1997	0404			
JP	200	05083	25	Τ		2000	0704		J:	P 19	97-5	3669	8	1997	0404			
TR	980	2042		Τ.	2	2000	0921		T	R 19	98-2	042		1997				
IN	199	7MA00	755	А		2005	0304		I	N 19	97-M	A755		1997	0410			
		3096												1997				
TW	419	465		В		2001	0121		$T^{\eta}$	W 19	97-8	6104	674	1997	0411			
BG	632	02		В	1	2001	0629		В	G 19	98-1	0277	0	1998	0915			
							0815			S 19	98-1	5594	8	1998	1008			
NO	980	4713		А		1998	1009		N	0 19	98 - 4	713		1998	1009			
NO	311	802		В	1	2002	0128											
KR	200	00053	66	Α		2000	0125		K.	R 19	98-7	0808	8	1998	1010			
RIORIT	Y API	PLN.	INFO	.:					D:	E 19	96-1	9614.	542	1996	0412			
									M	0 19	97-E	P168	7	1997	0404			

OTHER SOURCE(S): CASREACT 127:346409

$$R^6 Z C R^4 R^5 C H R O$$
 $X$ 
 $R^3$ 
 $R^3$ 

Title compds. [I; R = tetrazolyl, cyano, acyl; R2 = H, OH, amino, halo, alkyl, haloalkyl, alkoxy, haloalkoxy, alkylthio, etc.; R3 = H, OH, amino, halo, alkyl, haloalkyl, alkoxy, haloalkoxy, alkoxyamino, alkylthio, etc.; R4, R5 = (substituted) Ph, naphthyl; R6 = H, (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, Ph, naphthyl, heteroaryl; X = N, CR12; R12 = H, alkyl; R2R12 or R3R12 = alkylene, alkenylene; Y = N, CH, Z = O, S], were prepared Thus, Me 2-hydroxy-3-methoxy-3,3-diphenylpropionate (preparation given), 2,6-dimethoxy-4-chloropyrimidine, and K2CO3 were stirred at 100° in DMF to give Me 2-(2,6-dimethoxypyrimidin-4-yloxy)-3-methoxy- 3,3-diphenylpropionate. I bound to ETA receptors with Ki = 0.038-3.3  $\mu$ M.

MSTR 1

```
G1 = tetrazolyl
```

G40 = Ph (opt. substd. by 1 or more G41)

G41 = halo

G44 = 0

G45 = alkenyl < containing 3-6 C >

(opt. substd. by 1 or more G46)

G46 = halo / Ph (opt. substd. by 1 or more G51)

Patent location: claim 1

Note: additional ring formation also claimed

L89 ANSWER 26 OF 36 MARPAT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 127:346399 MARPAT Full-text

ACCESSION NOMBER: 127:340399 MARPAI EULI-CEXT

TITLE: Preparation of 1-(3-substituted-1,2,5-thiadiazol-4-yl)-

4-azatricyclo[2.2.1.02,6]heptanes for treating CNS

disorders

INVENTOR(S): Jeppesen, Lone; Olesen, Preben H.; Sauerberg, Per

PATENT ASSIGNEE(S): Novo Nordisk A/S, Den. SOURCE: PCT Int. Appl., 46 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

		TENT											ON N		DATE				
		9736													1997	0402			
		W:	AL,	ΑM,	ΑT,	ΑU,	ΑZ,	ΒA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CU,	CZ,	DE,	
			DK,	EE,	ES,	FΙ,	GB,	GE,	GH,	HU,	IL,	IS,	JP,	KE,	KG,	ΚP,	KR,	KΖ,	
			LC,	LK,	LR,	LS,	LT,	LU,	LV,	MD,	MG,	MK,	MN,	MW,	MX,	NO,	NZ,	PL,	
			PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	ТJ,	TM,	TR,	TT,	UA,	UG,	UZ,	VN,	YU
		RW:	GH,	ΚE,	LS,	MW,	SD,	SZ,	UG,	ΑT,	BE,	CH,	DE,	DK,	ES,	FΙ,	FR,	GB,	
			GR,	ΙE,	ΙΤ,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	
			ML,	MR,	ΝE,	SN,	TD,	ΤG											
	US	5914	338		Α		1999	0622		U	S 19	97-8	3135	8	1997	0401			
	IN	1997	MA00	679	А		2005	0304		I	N 19	97-M	A679		1997	0401			
	ZA	9702	790		Α		1997	1002		$Z_{2}$	A 19	97-2	790		1997	0402			
	CA	2250	843		Α	1	1997	1009		C	A 19	97-2	2508	43	1997	0402			
	ΑU	9722	871		А		1997	1022		A	U 19	97-2	2871		1997	0402			
	ΕP	8913	63		Α	1	1999	0120		E.	P 19	97-9	1535	4	1997	0402			
	EP	8913	63		В	1	2003	0827											
		R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙΤ,	LI,	LU,	NL,	SE,	MC,	PT,	
			ΙE,	FI															
	JP	1150	9864		Τ		1999	0831		J.	P 19	97-5	3484	4	1997	0402			
	JP	3162	727		В	2	2001	0508											
	ΑT	2481	72		Τ		2003	0915		A	T 19	97-9	1535	4	1997	0402			
PRIO:	RIT	Y APP	LN.	INFO	.:					D:	K 19	96-3	77		1996	0402			
										D:	K 19	96-1	281		1996	1114			
										M	0 19	97-D	K142		1997	0402			
GI																			

The title compds. [I; R = H, halo, C3-8 cycloalkyl, etc.] and their salts, useful in treating a disease in the central nervous system caused by malfunctioning of the muscarinic cholinergic system, were prepared and formulated. Thus, reduction of 1-cyano-4-azatricyclo[2.2.1.02,6]heptane with DIBAL-H in THF followed by treatment of the resulting 1-formyl-4-azatricyclo[2.2.1.02,6]heptane with KCN in H2O, reaction of the resulting cyanohydrin with NH4Cl in ammonia aqueous solution, cyclization of 2-amino-2-(4-azatricyclo[2.2.1.02,6]hept-1-yl)acetonitrile with sulfur monochloride in DMF, and reaction of 1-(3-chloro-1,2,5-thiadiazol-4-yl)-4-azatricyclo[2.2.1.02,6]heptane with 1-Pr bromide afforded I.oxalate [R = Pr] which showed IC50 of 4.3 nM against specific binding of 3H-Oxo.

$$\mathbb{G}_{\mathbb{N}}$$

G1

```
165—66 187—68 297—611—67—613 287—611—614
 3 G 7 --- G 1 5 -- G 1 6
G2
       = F / Ph (opt. substd. by 1 or more G9)
G6
       = carbon chain < containing 1-15 C,
         0 or more double bonds, 0 or more triple bonds>
         (opt. substd. by 1 or more G2)
G7
       = 0
G9
      = F
G11
      = carbon chain <containing 1-15 C,
        0 or more double bonds, 0 or more triple bonds>
        (opt. substd. by 1 or more G12)
G12
      = CF3 / CN / Ph (opt. substd. by 1 or more G9)
G14
     = 31
 3 G 7 --- G 6
```

Patent location: claim 1

= 16 / 18 / 24 / 28 / 33

L89 ANSWER 27 OF 36 MARPAT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 125:58749 MARPAT Full-text

TITLE: High activity ruthenium or osmium metal carbene

complexes for olefin metathesis reactions and

synthesis thereof

INVENTOR(S): Grubbs, Robert H.; Nguyen, Sonbinh T.; Johnson, Lynda

K.; Hillmyer, Marc A.; Fu, Gregory C.

PATENT ASSIGNEE(S): California Institute of Technology, USA

SOURCE: PCT Int. Appl., 27 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PA:	MG, TM, RW: KE, LU, SN, CA 2196061 CA 2196061 AU 9532728 AU 691645 EP 773948 R: AT, JP 09512828 JP 3067031 JP 3067031 EP 1251135 EP 1251135			KII	MD	DATE			AI	PPLI	CATI	ON N	Ο.	DATE				
WO.	9604	1289		Δ.	 1	1996	0215		 W.	19	 95-11	 5965	 5	1995	1728			
,,,			AT.													ES.	FT.	
														LT,				
				,	,	210,	,	,	,	1.0,	1.0,	02,	<i>,</i>	00,	O = 1	221,	,	
	RW:	•		SD,	SZ,	UG,	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IE,	IT,	
		•	•	•	•	•	•	•	•	•	•		,	GN,	•	•	•	
			TD,		·	·	·	·	•	·	·	·	·	·	·	·	·	
CA	2196		·	A.	1	1996	0215		CZ	A 199	95-2	1960	61	19950	0728			
CA	2196	061		С		2000	0613											
AU	9532	2728		Α		1996	0304		ΑU	J 19	95-3	2728		19950	0728			
AU	6916	45		В	2	1998	0521											
EP	7739	48		A	1	1997	0521		EI	9 19	95-9	2934	0	1995	728			
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙE,	ΙΤ,	LI,	LU,	MC,	NL,	PT,	SE
JP	0951	2828		T		1997	1222		JI	9 19	95-5	0667	6	19950	728			
JP	3067	7031		В	2	2000	0717											
JP	3067	7031		B.	2	2000	0717		JI	9 19	96-5	0667	6	1995	728			
EP	1251	.135		A.	2	2002	1023		EF	20	02-1	6470		1995	728			
EP	1251	.135		A.	3	2004	0102											
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙT,	LI,	LU,	NL,	SE,	MC,	PT,	ΙE
EP	1253	3156		A.	2	2002	1030		EI	20	02-1	6469		1995	728			
EP	1253	3156		Α.	3	2004	0107											
			BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙT,	LI,	LU,	NL,	SE,	MC,	PT,	ΙE
				А		1999	0309		U:	5 19	95-5	4844	5	1995	1026			
				А		1999	0713					4891		1995	1026			
				А		1998						5030		1995				
						1998						0506		1996				
				А		1998						0805		1996				
				А		1999						6261		1997				
				А		1998						6996		1997				
				A		1999			JI	? 19	98-2	5694.	3	1998	0910			
				B:	2	2002	1203						_					
PRIORIT	y ape	·LN.	INFO	.:								8282		1994				
												8282		1994				
												6360		19920				
												0629		19930				
												2934		1995				
												0667		1995				
												S965		19950				
												4844		1995				
OTHER OF	711D @ F	1 ( 0 )			070	ייסיקורי	T 10	E . E O '		5 I9!	ソコーち	5067	9	1995	TCOT			
OTHER SO	JUKCE	1(2):			CAS	REAC'	1 12:	);	149									
GI																		

AB Ru and Os carbene compds. which are stable in the presence of a variety of functional groups and which can be used to catalyze olefin methathesis reactions are discussed. Methods for synthesizing these carbene compds. are also disclosed. For example, 1.73 mmol [(cymene)RuCl2]2, 2 equiv PCy3 and 1

equiv 3,3-diphenylcyclopropene react in benzene at 83-85° for 6 h to give 88% Cl2Ru(:CHCH:CPh2)(PCy3)2 (I). Phosphoranes, R4R5R6P:CRR1, can be used in place of cyclopropenes. Specifically, the present invention relates to carbene compds. I wherein: M is Os or Ru; R and R1 are independently selected from H; C2-C20 alkenyl, C2-C20 alkynyl, C1-C20 alkyl, aryl, C1-C20 carboxylate, C2-C20 alkoxy, C2-C20 alkenyloxy, C2-C20 alkynyloxy, aryloxy, C2-C20 alkoxycarbonyl, C1-C20 alkylthio, C1-C20 alkylsulfonyl or C1-C20 alkylsulfinyl; each optionally substituted with C1-C5 alkyl, halogen, C1-C5 alkoxy or with a Ph group optionally substituted with halogen, C1-C5 alkyl or C1-C5 alkoxy; X and X1 are independently selected from any anionic ligand; and L and L1 are each trialkylphosphine ligands where at least one of the alkyl groups on the phosphine is a secondary alkyl or a cycloalkyl. In a preferred embodiment, all of the alkyl groups of the trialkylphosphine are either a secondary alkyl or a cycloalkyl. In a more preferred embodiment, the alkyl groups are either iso-Pr, iso-Bu, sec-Bu, neopentyl, neophenyl, cyclopentyl or cyclohexyl. Reactions catalyzed by the above complexes include ring-opening metathesis polymerization of strained and unstrained cyclic olefins, ring closing metathesis of acyclic dienes, cross metathesis reactions involving at least one acyclic or unstrained cyclic olefin and depolymn. of olefinic polymers. For example, 0.50 mmol CH2:CHCH2OCHPhCH2CH:CH2 was converted in 86% yield to the dihydropyran in benzene in the presence of I after 5 h at 20°. Telechelic polymers can be prepared using the above complexes as catalysts.

MSTR 1

$$\begin{array}{c}
G3 \\
G3
\end{array}$$

$$\begin{array}{c}
G4 \\
G1 \\
G4
\end{array}$$

G2 = alkenyloxy <containing 2-20 C> (opt. substd. by 1 or more G24) G23 = 204



Note: additional ring formation specified

L89 ANSWER 28 OF 36 MARPAT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 125:58534 MARPAT <u>Full-text</u>

TITLE: Preparation of pyrimidine- and triazine-derivative

endothelin receptor antagonists

INVENTOR(S): Riechers, Hartmut; Klinge, Dagmar; Amberg, Wilhelm;

Kling, Andreas; Mueller, Stefan; Baumann, Ernst;

Rheinheimer, Joachim; Vogelbacher, Uwe Josef; Wernet,

Wolfgang; et al.

PATENT ASSIGNEE(S): BASF A.-G., Germany SOURCE: Ger. Offen., 28 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PA:	TENT NO.		KIND	DATE		APP	LICAT	ION NO.	DATE		
DE	19533023		A1	19960418		DE	1995-	19533023	3 19950907		
DE	19533023		B4	20070516					19951007		
CA	2201785		A1	19960425		CA	1995-	2201785	19951007		
CA	2201785		C	20060829							
WO									19951007		
					CZ,	FI, H	W, JP	, KR, K	z, MX, NO,	NZ,	PL,
		•	· ·	, UA, US					_		
									J, MC, NL,		SE
AU	9538045		Α	19960506		AU	1995-	38045	19951007		
AU	688611		B2	19980312					19951007		
EP	785926		A1	19970730		EP	1995-	935916	19951007		
EP	785926		B1	20010822							
	R: AT,	BE,	CH, DE,	, DK, ES,	FR,	GB, G	R, IE	, IT, LI	[, LU, NL,	PT,	SE
CN	1160396		A -	19970924		CN	1995-	195655	19951007 19951007		
BR	9509338		Α	19971104		BR	1995-	9338	19951007		
HU	77443		A2	19980428		HU	1997-	1975	19951007		
HU	220621		B1	20020328							
JP	10507190		T	19980714		JP	1996-	512911	19951007		
JP	3957748		B2	20070815					19951007		
EP	1110952		A1	20010627		EP	2001-	103889	19951007		
	R: AT,	BE,	CH, DE,	, DK, ES,	FR,	GB, G	R, IT	, LI, LU	J, NL, SE,	PT,	ΙE
AT	204568		T	20010915		AT	1995-	935916	19951007 19951007		
ES	2162942		T3	20020116		ES	1995-	935916	19951007		
PI	785926		7	20020228		PT	1995-	935916	19951007		
RU	2180335		C2	20020310		RU	1997-	10/61/	19951007		
PL	186850		BI	20040331		PL	1995-	319655 1000370	19951007		
CN	1513844		A	20040721		CN	2004-	10002/83	19951007 3 19951007 19951007 19951007 19951007		
AI	2//911		I DC	20041015		A1	2001-	103889	19951007		
C Z	294603		E0	20050216		CZ EC	1997-	102000	19951007		
ES	2220990		1.3	20030401		ES	2001-	1000005	19951007		
CN	1923820		A	20070307		CN	2006-	115560	19951007		
ΤL	113360		A	20030212		7 L	1995-	113360	19951011		
пк	930317		BT.	20040630		HK TG	1995-	O 4 1 1 0 0 0 0	19951013		
TW	5//880		В	20040301		T M	1995-	84110900	19951017 19970327		
							1997-				
	9701529 9701675		A	19970411			1997-		19970411		
	308846		A B1	19970610 20001106		NO	エンフィー	TO 13	19970411		
	5969134			19991019		TTC	1990	184152	19981102		
	6197958		A B1	20010306				309770	19981102		
	200200524	105	A1	20010306				748184	20001227		
	6600043	±ツン	B2	20020502		US	2000-	140104	2000122/		
	3036931		В2 Т3	20030729		CD	2001	401798	20011018		
ЭĽ	2020321		10	20020131		GK	2001-	401/20	20011010		

	7109205	В2	20060919	US	2003-602275	20030624
US	20040092742	A1	20040513			
HR	2004000364	B1	20060930	HR	2004-364	20040422
HK	1066541	A1	20070601	HK	2004-109463	20041201
US	20060160808	A1	20060720	US	2006-377879	20060316
US	7119097	B2	20061010			
US	20060276645	A1	20061207	US	2006-502257	20060810
US	20060276474	A1	20061207	US	2006-502293	20060810
JP	2007126488	A	20070524	JP	2007-40759	20070221
JP	2007137892	A	20070607	JP	2007-40760	20070221
JP	2007137893	A	20070607	JP	2007-40761	20070221
JP	2007169295	A	20070705	JP	2007-40758	20070221
US	20070203338	A1	20070830	US	2007-789630	20070425
PRIORIT	Y APPLN. INFO.:			DE	1994-4436851	19941014
				DE	1995-19533023	19950907
				CN	2004-10002783	19951007
				EP	1995-935916	19951007
				JP	1996-512911	19951007
				WO	1995-EP3963	19951007
				US	1997-809699	19970327
				US	1998-184152	19981102
				US	1999-309770	19990511
				US	2000-748184	20001227
				US	2003-602275	20030624
				US	2006-502257	20060810
		~-		E 0 E 0 4		

OTHER SOURCE(S): CASREACT 125:58534

GΙ

The title compds. [I; R = CHO, tetrazolyl, CN, CO2H, groups cleavable to CO2H; AΒ R2 = (un)substituted NH2, halogen, (un)substituted alkyl, etc.; R3 = H, OH, (un) substituted NH2, halogen, (un) substituted alkyl, etc.; R4, R5 = (un) substituted Ph or naphthyl; R6 = H, alkyl, alkenyl, alkynyl, alkylcarbonyl, (un)substituted Ph, etc.; X = N, (un)substituted CH; Y = direct bond, S, O; Z = S, O, SO, SO2, direct bond], useful as endothelin receptor antagonists, are prepared Thus, pyrimidine derivative II, m.p. 167°, demonstrated a Ki ETA of 6 nM.

MSTR 1A

= tetrazolyl G13 = Ph (opt. substd. by 1 or more G14) G14 = halo = alkenyl <containing 3-6 C> G26 (opt. substd. by 1 or more G27) G27 = halo / Ph (opt. substd. by 1 or more G28) G33 = 0 G34 = 0 Patent location: Note: substitution is restricted

L89 ANSWER 29 OF 36 MARPAT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 123:307319 MARPAT <u>Full-text</u>

TITLE: Carboxylic acid derivatives as inhibitors of

endothelin binding to receptors

INVENTOR(S): Baumann, Ernst; Vogelbacher, Uwe Josef; Rheinheimer,

Joachm; Klinge, Dagmar; Riechers, Hartmut; Kroeger, Burkhard; Bialojan, Siegfried; Bollschweiler, Claus;

Wernet, Wolfgang; et al.

PATENT ASSIGNEE(S): BASF A.-G., Germany SOURCE: Ger. Offen., 31 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PAI	ENT I	NO.		KII	MD	DATE			Al	PPLI	CATI	и ис	Ο.	DATE				
DE	4411:	 225			 1	19951005				 : 19	94-4	4112	19940331					
HR	9501	15		B	- 1	20011231			HR 1995-115					19950309				
						19951012												
CA	2186	784		С		2007	0220											
WO	9526	716		A	1	1995		M	) 19	95-E	P109	9	1995					
														NO,			RU,	
				UA,		·	•	·	·	·	·	·	·	,	·	·	·	
	RW:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE	
AU	9521	356		A		1995	1023		Αl	J 19	95-2	1356		1995	0323			
AU	6951	93		В	2	1998	0806							1995				
EP	7528.	54		A.	1	1997						19950323						
EP	7528	54		В	1	2001	0822											
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙE,	ΙT,	LI,	LU,	NL,	PT,	SE	
CN	1148	807		А		1997	0430		CI	1 19	95-19	9316	7	1995	0323			
CN	1070	701		В	A 19970430 B 20010912													
HU	7530.	5		A:	2	19970528			HU 1996-2695					19950323				
BR	9507	231		Α		19970916			BR 1995-7231 JP 1995-525391					19950323				
JP	0951	0984		Τ		1997	1104		JI	9	95-5	2539	1	19950323				
JP	4001	622		B.	2	2007	1031											
PL	1795	80		В	1	2000	0929		Pl	L 19	95-3	1656	3	19950323				
	2163					2001								1995	0323			
ΑT	2044	71		Τ		2001	0915		A.	Г 19	95-9	1430	1	1995				
	2162	916		T	3	2002	0116		$\mathbf{E}_{i}^{s}$	5 19	95-9	1430	1	1995				
	7528.													1995				
CZ	2906	84		В	6	2002	0911		C:	Z 19	96-2	873		1995	0323			
	1131	37		А		1999	1028		I	L 19	95-1	1313	7	1995	0327			
	3825	94		В		2000	0221		TI	√ 19	95-8	4103	012	1995	0328			
ZA	9502	614		A		1996	0930		$Z_{I}$	A 19	95-2	614		1995 1996	0330			
FI	9603	885		А		1996	1126		F	I 19	96-3	885		1996	0927			

FI	118589	В1	20080115			
NC	9604121	A	19961126	ИО	1996-4121	19960927
NC	310497	B1	20010716			
US	5840722	A	19981124	US	1996-718377	19960930
GF	3036606	Т3	20011231	GR	2001-401467	20010912
JF	2007131645	A	20070531	JΡ	2007-34659	20070215
PRIORIT	Y APPLN. INFO.:			DE	1994-4411225	19940331
				JΡ	1995-525391	19950323
				WO	1995-EP1099	19950323

GΙ

$$R^{6}ZC(R^{4})(R^{5})CH(R)Y$$
 $N$ 
 $X$ 
 $R^{3}$ 

Carboxylic acid derivs. I [R = CHO, CO2H, group hydrolyzable to CO2H; R2, R3 = AΒ halo, C1-4 alkyl, C1-4 alkoxy, C1-4 haloalkoxy, C1-4 alkylthio; X = N, CR14; R4 = (substituted) C1-10 alkyl, (substituted) C3-12 cycloalkyl or cycloalkenyl, (substituted) C3-6 alkenyl or alkynyl, (substituted) heterocyclyl, (substituted) Ph or naphthyl; R5 = H, (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, or R4 and R5 complete a 3-8-membered ring; R6 = (substituted) alkyl, (substituted) alkenyl, (substituted) alkynyl, (substituted) cycloalkyl; R14 = H or forms an O-containing 3-4-membered alkylene or alkenylene chain with R3; Y = S, O, single bond; Z = S, O] are prepared as inhibitors of endothelin binding to receptors for treatment of e.g. (pulmonary) hypertension, acute myocardial infarct, Raynaud's syndrome, Me, R6 = 4-isopropylphenyl, X = CH, Y = Z = O) inhibited binding of endothelin to endothelin A receptors of cloned human CHO cells and endothelin B receptors of guinea pig cerebellar membranes with Ki  $2.5 \times 10^{-7}$  and  $3.0 \times 10^{-6}$ M, resp. I (R = CO2Me, R2 = R3 = OMe, R4 = R6 = Ph, R5 = H, X = CH, Y = S, Z = O) was prepared by reaction of Me 3-phenoxy-3-phenyl-2-hydroxybutyrate (preparation given) with MeSO2C1 and 4,6-dimethoxypyrimidine-2-thiol.

MSTR 1

G3 = 6



G4 = N G9 = 36



G10 = Ph (opt. substd. by 1 or more G16)

G16 = halo

G18 = alkyl <containing 1-3 C>

(substd. by alkoxy <containing 1-3 C>)

G26 = alkenyl <containing 3-6 C>

(opt. substd. by 1 or more G27)

G27 = halo / Ph (opt. substd.)

G43 = 0

Patent location: claim 1

Note: substitution is restricted

L89 ANSWER 30 OF 36 MARPAT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 122:161364 MARPAT  $\underline{\text{Full-text}}$ 

TITLE: Preparation of N-acyl  $\beta$ -amino acid derivatives as

platelet aggregation inhibitors Tjoeng, Foe S.; Toth, Mihaly V.

PATENT ASSIGNEE(S): G.D. Searle and Co., USA; Monsanto Co.

SOURCE: PCT Int. Appl., 34 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

INVENTOR(S):

PA	PATENT NO.				KIND DATE				Α.	PPLI	CATI	Э.	DATE				
WO	WO 9420457			A	A1 19940915				M	) 19	94-U	4	19940222				
	W:	ΑT,	ΑU,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CZ,	DE,	DK,	ES,	FΙ,	GB,	HU,
		JP,	KP,	KR,	KΖ,	LK,	LU,	LV,	MG,	MN,	MW,	NL,	NO,	NZ,	PL,	PT,	RO,
		RU,	SD,	SE,	SK,	UA,	US,	UZ,	VN								
	RW:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,
		BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	ML,	MR,	NE,	SN,	TD,	ΤG		
AU	9462	678		А		1994	0926		AU 1994-62678 19940222								
US	5710	166		A		1998	0120		U	S 19	95-5	1866	0	1995	0824		
PRIORIT	Y APP	LN.	INFO	.:					U	S 19	93-2	4977		1993	0302		
									M	0 19	94-U	S159	4	1994	0222		

GΙ

Title compds. I (R = H, alkyl, alkenyl, alkynyl, acyclyl, and aromatic all optionally substituted, (substituted)heterocyclyl; A = alkyl, alkenyl, alkynyl, alicyclyl, heterocyclyl, aryl all optionally substituted; W = H, alkyl, alkenyl, alkynyl, alicyclyl, aromatic all optionally substituted; Z, Z' = H, alkyl, halo, alkoxy, NC, SO2, HO; m = 0-6; n = 0-3) or a pharmaceutically acceptable salt, are prepared 4-Cyanobenzaldehyde, 3-aminobenzoic acid and NaBH3CN were reacted tp give 3-(4- cyanobenzyl)aminobenzoic acid which was reacted with  $\beta$ -alanine Et ester-HCl, EtN(Me2CH)2 and (benzotriazol-1- yloxy)tris(dimethylamino)phosph onium hexafluorophosphate to give Et  $\beta$ -[[3-[4(aminoiminomethyl)benzyl]aminobenzoyl]amino]propanoate which was treated with 1N LiOH and MeOH to give the title compound II. In vitro platelet aggregation inhibition in platelet-rich plasma in dog of II was IC50 = 28% at 10-5M.

MSTR 1

```
= alkyl <containing 1-10 C>
G1
         (opt. substd. by 1 or more G2)
       = alkyl <containing 1-10 C> / F / CO2H / CF3 /
G2
        Ph (opt. substd. by 1 or more G3)
G3
       = F
G8
       = 13
 19-----G9
G9
       = alkenyl <containing 2-10 C>
         (opt. substd. by 1 or more G2)
G12
```

G13 = (0-6) CH2

G16 = alkoxy <containing 1-10 C>

Derivative: or pharmaceutically acceptable salts

Patent location: claim 1

L89 ANSWER 31 OF 36 MARPAT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 122:31550 MARPAT Full-text

TITLE: Preparation of 3-(hetero)arylcarboxylic

acid-derivative herbicides with increased species

selectivity

INVENTOR(S): Baumann, Ernst; Rheinheimer, Joachim; Vogelbacher, Uwe

Josef; Bratz, Matthias; Theobald, Hans; Gerber, Matthias; Walter, Helmut; Rademacher, Wilhelm;

Westphalen, Karl Otto

PATENT ASSIGNEE(S): BASF A.-G., Germany SOURCE: Ger. Offen., 25 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PAT	TENT NO.		KIND DATE			API	DATE							
DE	4313412		A1	19941027 19941110		DE	 1993-4	  31341	.2	19930	0423			
CA	2160912		A1	19941110		CA	1994-2	16091	.2	19940	0413			
CA	2160912		С	20071002										
WO	9425442		A1	19941110		WO	1994-E	P1141		19940	)413			
	W: AU,	BR, E	BY, CA	, CN, CZ,	FI,	HU, 3	JP, KR,	KΖ,	NO,	NZ,	PL,	RU,	UA,	US
	RW: AT,	BE, C	CH, DE	, DK, ES,	FR,	GB, (	GR, IE,	ΙΤ,	LU,	MC,	NL,	PT,	SE	
AU	9465681		A	19941121		AU	1994-6	5681		19940	0413			
AU	678236		B2	19970522										
BR	9406478		A	19960102		BR	1994-6	478		19940	0413			
EP	695295		A1	19960102 19960207		EP	1994-9	13588	3	19940	0413			
EP	695295		В1	20020306										
	R: AT,	BE, C	CH, DE	, DK, ES,	FR,	GB, (	GR, IE,	ΙΤ,	LI,	LU,	NL,	PT,	SE	
CN	1121711		A	19960501		CN	1994-1	91867	7	19940	0413			
CN	1066141		В	19960501 20010523 19960828										
HU	73558		A2	19960828		HU	1995-3	040		19940	)413			
HU	221475		В	20021028 19960917 20040106										
JP	08508723		T	19960917		JP	1994-5	21408	3	19940	0413			
JP	3483254		B2	20040106										
RU	2140413		C1	19991027		RU	1995-1	.20099	)	19940	)413			
PL	179463		B1	20000929		PL	1994-3	11228	3	19940	)413			
AT	214053		Τ	20020315		AT	1994-9	13588	3	19940	0413			
PT	695295		T	20000929 20020315 20020830 20021101		PT	1994-9	13588	}	19940	0413			
ES	2173916		Т3	20021101		ES	1994-9	13588	}	19940	0413			
CZ	291468		В6	20030312		CZ	1995-2	768		19940	0413			
FI	9504994		A	20021101 20030312 19951019		FΙ	1995-4	1994		19951	1019			
FΙ	113650		В1	20040531										
US	5703017		A	19971230		US	1995-5	37843	}	19951	1019			
NO	9504211		A	19951220 20000207		ИО	1995-4	211		19951	1020			
				20000207										
PRIORITY	Y APPLN.	INFO.:					1993-4							
						WO	1994-E	P1141		19940	0413			

GΙ

The title compds. [I; R1 = H, succinylimidoxy, (un)substituted N-containing 5-member heterocyclic group, etc.; R2, R3 = halogen, C1-4 alkyl or alkoxy or alkylthio, etc.; R4 = (un)substituted Ph, (un)substituted naphthyl, (un)substituted heteroarom. residue, etc.; R5 = H, alkyl, alkenyl, alkynyl, cycloalkyl, Ph, etc.; R6 = (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl; X = N, (un)substituted CH; Y = direct bond, O, S; Z = O, S], useful as herbicides which have reduced toxicity com. plant species, are prepared Thus, pyrimidine derivative II (m.p. 165°; decomposition) was prepared and demonstrated 10% plant loss when applied to Gossypium hirsutum (i.e., cotton) at 0.125 kg/ha, vs. 35% plant loss for a control experiment using I (R1 = OH, R2 = R3 = OMe, R4 = Ph, R5 = R6 = Me, X = CH, Y = Z = O).

MSTR 1

$$G34 = N$$
 $G35 = 6$ 

```
G38
       = Ph (opt. substd. by 1 or more G48)
G40
       = alkyl <containing 1-4 C>
         (substd. by alkoxy <containing 1-4 C>)
G41
       = bond
G42
      = 0
G48
       = halo
       = alkenyl <containing 3-6 C>
G49
         (opt. substd. by 1 or more G50)
       = halo / Ph (opt. substd. by 1 or more G51)
G50
Patent location:
                            claim 1
                            substitution is restricted
Note:
```

L89 ANSWER 32 OF 36 MARPAT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 119:138791 MARPAT Full-text

TITLE: Cyclohexenone derivatives and their use as herbicides

and plant growth regulators

INVENTOR(S): Kast, Juergen; Zierke, Thomas; Bratz, Matthias;

Misslitz, Ulf; Meyer, Norbert; Landes, Andreas; Rademacher, Wilhelm; Westphalen, Karl Otto; Walter,

Helmut

PATENT ASSIGNEE(S): BASF A.-G., Germany SOURCE: Ger. Offen., 18 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PAT	FENT 1	NO.		KII	ND.	DATE			AP:	PLIC	CATI	DATE				
	DE	4135265			 A:	1	1993	0429		DE	199	1-4	19911025				
	WO	9308	9308153			1	19930429			WO	199	2-E	P222	6	1992		
		W:	ΑU,	BR,	CA,	CS,	HU,	JP,	KR,	PL,	RU,	US					
		RW:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	SE
	AU	9226	482		А		1993	0521		AU	199	2-2		19920926			
	AU	6620	18		B	B2 19950817											
	ΕP	6092	59		A.	1	1994	0810		EP	199	2-9:	2069	1	1992	0926	
	ΕP	6092	59		B1 19951122												
		R:	ΑT,	BE,	CH,	DE,	ES,	FR,	GB,	IT,	LI,	NL					
	JP	0750	0821		T		1995	0126		JP	199	2-5	0737	9	1992	0926	
	ΑT	1305	96		T		1995	1215		ΑT	199	2-9:	2069	1	1992	0926	
	ES	2081	134		T	3	1996	0216		ES	199	2-9:	2069	1	1992	0926	
	US	5523	462		А		1996	0604		US	199	4-2	1181	9	1994	0419	
PRIO	RIT	Y APP	LN.	INFO	.:					DE	199	1 - 4	1352	65	1991	1025	
										WO	199	2-E	P222	6	1992	0926	

OTHER SOURCE(S): CASREACT 119:138791

GΙ

AB The title compds. I (R1 = alkyl, alkenyl, etc.; X, Y = alkoxy, hydroxy, amino, etc.; W = oxo or imino group) and their uses as herbicides or plant growth

regulators are claimed. More specifically, I are  $3-\infty-4-\text{cyclohexen-1},1-\text{dicarboxylates}$  or 3,5-dioxocyclohexane-1,1-dicarboxylates. Treatment of diet  $3-[(\text{cyclopropylcarbonyl})\,\text{oxy}]-5-\infty-3-\text{cyclohexene-1},1-\text{dicarboxylate}$  (II) with DMAP in methylene chloride gave di-Et 4-(cyclopropylcarbonyl)-3,5-dioxo-1,1-cyclohexanedicarboxylate (III).

MSTR 1

G4 = 14

1½—O—G5

G5 = 19

168-G10-G9

G12 = halo / Ph (opt. substd. by (1-3) G13) / 353

G23 N N

G13 = halo
Derivative:
Patent location:

and agriculturally acceptable salts and esters claim  $\ensuremath{\mathbf{1}}$ 

MSTR 3

$$G4 = 14$$

$$G5 = 19$$

MSTR 4

$$G5 = 19$$

G12 = halo / Ph (opt. substd. by (1-3) G13) / 303



G13 = halo

Patent location: claim 3

L89 ANSWER 33 OF 36 MARPAT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 118:102914 MARPAT Full-text

TITLE: Metallocenes containing ligands of 2-substituted

indenyl derivatives, process for their preparation,

and their use as polymerization catalysts

INVENTOR(S): Winter, Andreas; Antberg, Martin; Spaleck, Walter;

Rohrmann, Juergen; Dolle, Volker

PATENT ASSIGNEE(S): Hoechst A.-G., Germany SOURCE: Can. Pat. Appl., 31 pp.

CODEN: CPXXEB

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	API	PLICATION NO.	DATE
CA 2055218	A1	19920513	CA	1991-2055218	19911108
CA 2055218	С	20020903			
ES 2090209	Т3	19961016	ES	1991-118680	19911101
US 5276208	A	19940104	US	1991-789361	19911108
AU 9187760	A	19920514	AU	1991-87760	19911111
AU 640287	В2	19930819			
ZA 9108927	A	19920729	ZA	1991-8927	19911111
JP 06340684	A	19941213	JP	1991-294690	19911111
JP 3282839	В2	20020520			
US 37208	E1	20010605	US	1994-324260	19941017
US 39532	E1	20070327	US	1997-895909	19970717
US 39561	E1	20070410	US	1997-895950	19970717
US 37573	E1	20020305	US	1999-252719	19990219
PRIORITY APPLN. INFO.	:		DE	1990-4035884	19901112
			US	1991-789361	19911108
			DE	1992-4225649	19920803
			US	1993-101408	19930803
			US	1994-324260	19941017

Olefins, especially C3H6, are stereospecifically polymerized using the title catalysts to give polymers with high crystallinity, hardness and m.p., useful as engineering materials. Thus, C3H6 was polymerized using dimethyl(2-methyl-4,5,6,7-tetrahydro-1-indenyl)2zirconium dichloride and Me aluminoxane catalyst to give a polymer with isotactic index 96% and mol. weight 24,300.

MSTR 20

G15 = 0

G22 = alkylene <containing 1-2 C, unbranched>
 (opt. substd. by 1 or more G23)

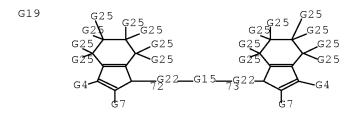
G23 = F / alkyl (opt. substd. by 1 or more G21) / alkoxy <containing 1-10 C> / alkenyl (opt. substd. by aryl) / Me / Ph / 161

Patent location: claim 4

Note: additional ring formation specified

Note: substitution is restricted

MSTR 3C



G15 = 0

G22 = alkylene <containing 1-2 C, unbranched>

(opt. substd. by 1 or more G23)

G23 = F / alkyl (opt. substd. by 1 or more G21) / alkoxy <containing 1-10 C> / alkenyl (opt. substd. by aryl) / Me / Ph / 161

Patent location: claim 4

Note: additional ring formation specified

Note: substitution is restricted

L89 ANSWER 34 OF 36 MARPAT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 117:213186 MARPAT Full-text

TITLE: Preparation of bisindene derivative metallocenes as

catalysts for polymerization of olefins

INVENTOR(S): Winter, Andreas; Antberg, Martin; Spaleck, Walter;

Rohrmann, Juergen; Dolle, Volker

PATENT ASSIGNEE(S): Hoechst A.-G., Germany SOURCE: Eur. Pat. Appl., 21 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATE	INT NO.	KIN	ND DATE	API	PLICATION NO.	DATE
EP 4	.85821 .85821 R: BE. [	A1 B1 DE. ES.		•	1991-118680	19911101
	090209	T3			1991-118680	19911101
US 5	276208	А	19940104	US	1991-789361	19911108
AU 9	187760	А	19920514	AU	1991-87760	19911111
AU 6	40287	B2	19930819	)		
ZA 9	108927	A	19920729	ZA	1991-8927	19911111
JP 0	6340684	A	19941213	JP	1991-294690	19911111
JP 3	282839	B2	2 20020520	)		
US 3	7208	E1	20010605	US	1994-324260	19941017
US 3	9532	E1	20070327	US	1997-895909	19970717
US 3	9561	E1	20070410	US	1997-895950	19970717
US 3	7573	E1	20020305	US	1999-252719	19990219
PRIORITY .	APPLN. IN	FO.:		DE	1990-4035884	19901112
				US	1991-789361	19911108
				DE	1992-4225649	19920803
				US	1993-101408	19930803
				US	1994-324260	19941017

AB Sandwich complexes of Group IVB, VB, or VIB metals with bisindenes of specified structure are catalysts for polymerization of olefins with high isotacticity and mol. weight The reaction of 2-methylindene, BuLi, and Me2SiCl2 in Et2O gave 52% (dimethylsilylene)bis(2-methylindene), reaction of which with BuLi and ZrCl4 in THF-CH2Cl2 gave 14% racemic complex which was hydrogenated over Pt in CH2Cl2 to give 60% 4,4',5,5',6,6',7,7'- octahydro derivative (I). Stirring 12 dm3 liquid C3H6 with 72 mmol (as Al) Me aluminoxane and 0.011 mmol I at 70° for 3 h gave polypropylene with productivity 50.3 kg/g I-h, weight-average mol. weight 24,300, polydispersity 2.4, isotactic index 96%, and m.p. 150°.

MSTR 2C

G15 = 0

G22 = alkylene <containing 1-2 C, unbranched>
 (opt. substd. by 1 or more G23)

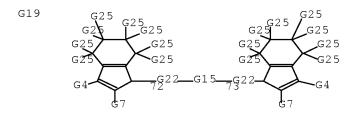
G23 = F / alkyl (opt. substd. by 1 or more G21) / alkoxy <containing 1-10 C> / alkenyl (opt. substd. by aryl) / Me / Ph / 161

Patent location: claim 4

Note: additional ring formation specified

Note: substitution is restricted

MSTR 3C



G15 = 0

G22 = alkylene <containing 1-2 C, unbranched>

(opt. substd. by 1 or more G23)

G23 = F / alkyl (opt. substd. by 1 or more G21) / alkoxy <containing 1-10 C> / alkenyl (opt. substd. by aryl) / Me / Ph / 161

Patent location: claim 4

Note: additional ring formation specified

Note: substitution is restricted

L89 ANSWER 35 OF 36 MARPAT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 117:131729 MARPAT Full-text

TITLE: Substituted bisindenyl-metallocenes, their preparation

and use as catalysts for the polymerization of

olefins

INVENTOR(S): Winter, Andreas; Antberg, Martin; Spaleck, Walter;

Rohrmann, Juergen; Dolle, Volker

PATENT ASSIGNEE(S): Hoechst A.-G., Germany SOURCE: Eur. Pat. Appl., 19 pp.

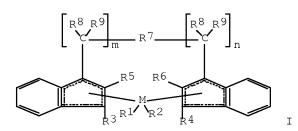
CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATI	ENT NO.		KIND	DATE			APE	PLICATION NO.	DATE
EP	 485823		A1	19920	520		EP	1991-118682	19911101
EP 4	485823		В1	19950	308				
	R: BE,	DE, E	S, FR,	GB,	ΙΤ,	NL			
ES 2	2071888		Т3	19950	701		ES	1991-118682	19911101
CA 2	2055219		A1	19920	513		CA	1991-2055219	19911108
CA 2	2055219		С	20020	806				
US !	5145819		A	19920	908		US	1991-790234	19911108
AU S	9187757		A	19920	514		AU	1991-87757	19911111
AU (	641341		B2	19930	916				
ZA S	9108926		A	19920	729		ZA	1991-8926	19911111
JP (	04300887	7	A	19921	023		JΡ	1991-294687	19911111
JP 3	3272005		B2	20020	408				
US 3	37384		E1	20010	918		US	1999-352824	19990713
PRIORITY	APPLN.	INFO.:					DE	1990-4035883	19901112
GI									



AB I (R1,R2 = H, organic group, halogen; R3,R4 = H, halogen, organic group optionally containing heteroatom; R5,R6 = as for R3, R4 but not H; R7 = organic or heteroatom-containing organic group; R8,R9,R10 = H, halogen, organic group; m,n = 0-2, with m + n = 0-2,; M = IVb, Vb, VIIb element) are obtained for use as catalysts, in conjunction with aluminoxanes, for the stereospecific polymerization of olefins. Thus, 1,2-ethenediylbis(2-methyl-1-

indene)zirconium dichloride (II) was obtained from the ligand and ZrCl4 in THF. Propylene (12 dm3) was mixed with 35 cm3 PhMe containing Me aluminoxane (52 mmol Al) and to this was added 6.9 mg II and Me aluminoxane (20 mmol Al) in PhMe and the mixture was heated at  $70^{\circ}$  to give 1.56 kg isotactic polypropylene (226 kg polymer/g II). Use of metallocenes unsubstituted in the 2-position of the indene ring resulted in lower mol. weight polymers.

MSTR 2C

G19
$$G_4$$
 $G_7$ 
 $G_7$ 

G15 = 0

G22 = alkylene <containing 1-2 C, unbranched>

(opt. substd. by 1 or more G23)

G23 = F / alkyl (opt. substd. by 1 or more G21) / alkoxy <containing 1-10 C> / alkenyl (opt. substd. by aryl) / Me / Ph / 161



Patent location: claim 4

Note: additional ring formation specified

Note: substitution is restricted

L89 ANSWER 36 OF 36 MARPAT COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 115:49729 MARPAT Full-text

TITLE: Preparation of substituted 2-pyrimidinyl and

2-triazinylacetic acid derivatives

INVENTOR(S): Harde, Christoph; Nordhoff, Erhard; Krueger, Anita; Krueger, Gabriele; Tarara, Gerhard; Wegner, Peter;

Heinrich, Nikolaus; Koetter, Clemens; Johann, Gerhard;

et al.

PATENT ASSIGNEE(S): Schering A.-G., Germany SOURCE: Eur. Pat. Appl., 27 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: German FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

EP	422751		A3	19910925					
EP	422751		B1	19960814					
	R: AT,	BE, C	CH, DE,	DK, ES,	FR,	GB, (	GR, IT, I	LI, LU,	NL, SE
DE	3934020		A1	19910418		DE	1989-393	34020	19891009
US	5098465		A	19920324		US	1990-590	0675	19901001
AT	141264		T	19960815		AT	1990-250	250	19901004
ES	2093632		Т3	19970101		ES	1990-250	250	19901004
JP	03169868	1	A	19910723		JP	1990-269	9690	19901009
US	5238907		A	19930824		US	1992-818	3518	19920109
PRIORITY	APPLN.	INFO.:				DE	1989-393	34020	19891009
						US	1990-590	0675	19901001

OTHER SOURCE(S): CASREACT 115:49729

GΙ

AB Title compds. [I; A = CO2R1, CONR6R7, cyano; R1 = H, (O- or S-interrupted) (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, dialkylmethyleneimino, cycloalkyleneimino; R2,R3 = alkyl, CF3, alkoxy, alkoxyalkyl, alkylthio, alkylamino, halo; R4 = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl; R5 = H, R4; R4R5C = cycloalkyl; R6,R7 = H, alkyl; X = N, CH], with restrictions, were prepared Thus, Me(CH2)3CO2Et in THF was added to (Me2CH)2NLi in THF at -60°; after 1 h 4,6-dimethoxy-2-methylsulfonylpyrimidine was added and the mixture was warmed to 10° over 2 h to give 42% title compound II. Several I at 0.3 kg/ha preemergent gave 90-100% damage on Bromus tectorum.

MSTR 1A

G2 = alkenyloxy <containing 3-8 C>
 (opt. substd. by 1 or more G8)

G8 = Ph / halo

G10 = 61

6 G 2 O-G 2 1

G11 = 61

6 G 2 O—G 2 1 G12 = 7 G13 = alkyl <containing 1-10 C> (opt. substd. by 1 or more G14) = 61 / Ph (opt. substd. by 1 or more halo) G14 6920—G21 G17 = N G20 = OPatent location: claim 1 alkoxy in G2 may be interrupted with oxygen or Note: sulfur atoms Note: substitution is restricted and optically active isomers Stereochemistry: MSTR 1B G2 = alkenyloxy <containing 3-8 C> (opt. substd. by 1 or more G8)

G2 = alkenyloxy  (opt. substd. by 1 or more G8)
$$G8 = Ph / halo$$

$$G10 = 61$$

$$6^{G20}-G21$$

G11 = 616 G 2 O—G 2 1

G17 = N

```
G13
     = alkyl <containing 1-10 C>
         (opt. substd. by 1 or more G14)
G14
      = 61 / Ph (opt. substd. by 1 or more halo)
 6 G 2 0 — G 2 1
G17 = N
G20
    = 0
Patent location:
                           claim 1
Note:
                            alkoxy in G2 may be interrupted with oxygen or
                            sulfur atoms
                            substitution is restricted
Note:
Stereochemistry:
                            and optically active isomers
 MSTR 1C
G2
      = alkenyloxy <containing 3-8 C>
         (opt. substd. by 1 or more G8)
G8
      = Ph / halo
G10
    = 61
 6 G 2 O-G 2 1
G11 = 61
 6 G 2 O - G 2 1
G13
     = alkyl <containing 1-10 C>
        (opt. substd. by 1 or more G14)
G14
      = 61 / Ph (opt. substd. by 1 or more halo)
 6 G 2 O-G 2 1
```

G19 = alkyl < containing 1-10 C>

(opt. substd. by 1 or more G14)

Patent location: claim 1

alkoxy in G2 may be interrupted with oxygen or sulfur atoms Note:

Note: substitution is restricted Stereochemistry: and optically active isomers

L12

9 SEA SSS SAM L11

```
=> d his full
     (FILE 'HOME' ENTERED AT 12:22:44 ON 16 APR 2008)
     FILE 'REGISTRY' ENTERED AT 12:22:53 ON 16 APR 2008
               STRUCTURE UPLOADED
L1
L2
              9 SEA SSS SAM L1
               D SCA
     FILE 'CAPLUS' ENTERED AT 12:24:39 ON 16 APR 2008
               E US2006-566911 /APPS
              1 SEA ABB=ON PLU=ON US2006-566911 /AP
L3
               D SCA
                SEL RN
     FILE 'REGISTRY' ENTERED AT 12:25:57 ON 16 APR 2008
           211 SEA ABB=ON PLU=ON (100-02-7/BI OR 100-39-0/BI OR 107714-87-4/
L4
                BI OR 110-87-2/BI OR 110-91-8/BI OR 1145-76-2/BI OR 126918-17-0
                /BI OR 127000-90-2/BI OR 133775-25-4/BI OR 133775-26-5/BI OR
               135206-87-0/BI OR 135270-08-5/BI OR 135272-36-5/BI OR 146500-63
                -2/BI OR 146500-65-4/BI OR 1608-24-8/BI OR 17392-83-5/BI OR
               1743-00-6/BI OR 1885-14-9/BI OR 1979-51-7/BI OR 1979-52-8/BI
               OR 1979-53-9/BI OR 1979-54-0/BI OR 207672-95-5/BI OR 210481-22-
                4/BI OR 210481-23-5/BI OR 212890-35-2/BI OR 220676-08-4/BI OR
                220676-10-8/BI OR 220676-12-0/BI OR 220676-13-1/BI OR 220676-14
               -2/BI OR 220676-15-3/BI OR 253266-68-1/BI OR 253266-69-2/BI OR
               253266-71-6/BI OR 253266-72-7/BI OR 253266-73-8/BI OR 28321-07-
               5/BI OR 28321-09-7/BI OR 286017-80-9/BI OR 288-88-0/BI OR
               348-57-2/BI OR 36029-95-5/BI OR 36029-97-7/BI OR 36029-98-8/BI
               OR 36030-01-0/BI OR 405-42-5/BI OR 492450-12-1/BI OR 51336-94-8
                /BI OR 52805-36-4/BI OR 616897-41-7/BI OR 6373-46-2/BI OR
               645-36-3/BI OR 678188-96-0/BI OR 74670-68-1/BI OR 767-00-0/BI
               OR 7785-11-7/BI OR 844877-73-2/BI OR 844877-76-5/BI OR
               844877-80-1/BI OR 844877-81-2/BI OR 844877-82-3/BI OR 844877-83
                -4/BI OR 844877-84-5/BI OR 844877-85-6/BI OR 844877-86-7/BI OR
               844877-87-8/BI OR 844877-88-9/BI OR 844877-89-0/BI OR 844877-90
               -3/BI OR 844877-91-4/BI OR 844877-92-5/BI OR 844877-93-6/BI OR
                844877-94-7/BI OR 844877-95-8/BI OR 844877-96-9/BI OR 844877-97
                -0/BI OR 844877-98-1/BI OR 844877-99-2/BI OR 844878-00-8/BI OR
               844878-01-9/BI OR 844878-02-0/BI OR 844878-03-1/BI OR 844878-04
               -2/BI OR 844878-05-3/BI OR 844878-06-4/BI OR 844878-07-5/BI OR
               844878-08-6/BI OR 844878-09-7/BI OR 844878-10-0/BI OR 844878-11
               -1/BI OR 844878-12-2/BI OR 844878-13-3/BI OR 844878-14-4/BI OR
               844878-15-5/BI OR 844878-16-6/BI OR 844878-17-7/BI OR 844878-18
                -8/BI OR 844878-19-9/BI OR 844878-20-2/BI OR 844878-21-3/BI OR
               844878
L5
           1000 SEA ABB=ON PLU=ON 84487!-?/RN
L6
           147 SEA ABB=ON PLU=ON L4 AND L5
L7
                STRUCTURE UPLOADED
L8
              9 SEA ABB=ON PLU=ON L2 AND L6
    FILE 'CAPLUS' ENTERED AT 12:36:18 ON 16 APR 2008
L9
              1 SEA ABB=ON PLU=ON L6
     FILE 'REGISTRY' ENTERED AT 12:36:23 ON 16 APR 2008
L10
             9 SEA SSS SAM L7
               STRUCTURE UPLOADED
L11
```

#### 10/566911 L13 STRUCTURE UPLOADED L14 11 SEA SSS SAM L13 D SCA D STAT QUE L14 L15 STRUCTURE UPLOADED 9 SEA SSS SAM L15 L16 L17 127 SEA SSS FUL L15 SAVE TEMP L17 RIC911STR15L/A FILE 'CAPLUS' ENTERED AT 12:46:41 ON 16 APR 2008 1 SEA ABB=ON PLU=ON L17 L18 FILE 'BEILSTEIN' ENTERED AT 12:46:53 ON 16 APR 2008 0 SEA SSS SAM L15 T.19 L20 0 SEA SSS FUL L15 FILE 'MARPAT' ENTERED AT 12:47:33 ON 16 APR 2008 L21 6 SEA SSS SAM L15 215 SEA SSS FUL L15 L22 SAVE TEMP L22 RIC911MARP/A L23 214 SEA ABB=ON PLU=ON L22/COM STRUCTURE UPLOADED L24 L25 1 SEA SUB=L22 SSS SAM L24 D SCA L26 1 SEA SUB=L22 SSS FUL L24 D SCA L27 STRUCTURE UPLOADED L28 12 SEA SUB=L22 SSS SAM L27 L29 STRUCTURE UPLOADED L30 1 SEA SUB=L22 SSS SAM L29 D SCA L31 STRUCTURE UPLOADED D STAT QUE L30 11 SEA SUB=L22 SSS SAM L31 L32 D SCA L33 STRUCTURE UPLOADED L34 11 SEA SUB=L22 SSS SAM L33 L35 STRUCTURE UPLOADED 11 SEA SUB=L22 SSS SAM L35 L36 STRUCTURE UPLOADED L37 L38 7 SEA SUB=L22 SSS SAM L37 D SCA D SCA L39 STRUCTURE UPLOADED L40 7 SEA SUB=L22 SSS SAM L39 L41 STRUCTURE UPLOADED L42 7 SEA SUB=L22 SSS SAM L41 D SCA L43 STRUCTURE UPLOADED L44 7 SEA SUB=L22 SSS SAM L43 L45 STRUCTURE UPLOADED L46 7 SEA SUB=L22 SSS SAM L45 D SCA L47 99 SEA SUB=L22 SSS FUL L45 STRUCTURE UPLOADED L48 L49 STRUCTURE UPLOADED STRUCTURE UPLOADED STRUCTURE UPLOADED L50 L51

L\*\*\* DEL 7 S L45 SAM SSS SUB=L22 L\*\*\* DEL STRUCTURE UPLOADED

```
L*** DEL
            7 S L52 SAM SSS SUB=L22
L52
              STRUCTURE UPLOADED
L53
             7 SEA SUB=L22 SSS SAM L52
L54
               STRUCTURE UPLOADED
L55
             5 SEA SUB=L22 SSS SAM L54
               D SCA
              STRUCTURE UPLOADED
L56
L57
               STRUCTURE UPLOADED
             1 SEA SUB=L22 SSS SAM L57
L58
               D SCA
L*** DEL
             2 S L57 FULL SSS SUB=L22
               STRUCTURE UPLOADED
L59
L60
             4 SEA SUB=L47 SSS SAM L59
                D SCA
L61
             23 SEA SUB=L47 SSS FUL L59
L62
            22 SEA ABB=ON PLU=ON L61/COM
L63
               STRUCTURE UPLOADED
L64
             1 SEA SUB=L22 SSS SAM L63
            20 SEA SUB=L22 SSS FUL L63
L65
            19 SEA ABB=ON PLU=ON L65/COM
L66
L67
               STRUCTURE UPLOADED
             1 SEA SUB=L22 SSS SAM L67
L68
               D SCA
               STRUCTURE UPLOADED
L69
             1 SEA SUB=L22 SSS SAM L69
L70
             17 SEA SUB=L22 SSS FUL L69
L71
L72
             17 SEA ABB=ON PLU=ON L71/COM
L73
             36 SEA ABB=ON PLU=ON L72 OR L62
                D COST
    FILE 'CAPLUS' ENTERED AT 14:20:02 ON 16 APR 2008
    15476 SEA ABB=ON PLU=ON KIM B?/AU
L74
          966 SEA ABB=ON PLU=ON MIN Y?/AU
L75
            0 S LEE Y?/AUY
L*** DEL
L76
         30107 SEA ABB=ON PLU=ON LEE Y?/AU
          1881 SEA ABB=ON PLU=ON PARK N?/AU
L77
          9952 SEA ABB=ON PLU=ON KIM W?/AU
            1 SEA ABB=ON PLU=ON L74 AND L75 AND L76 AND L77 AND L78
L79
            13 SEA ABB=ON PLU=ON L74 AND L75 AND L76 AND L77
1 SEA ABB=ON PLU=ON L74 AND L75 AND L76 AND L78
1 SEA ABB=ON PLU=ON L74 AND L75 AND L77 AND L78
L80
L81
L82
             1 SEA ABB=ON PLU=ON L74 AND L76 AND L77 AND L78
L83
             1 SEA ABB=ON PLU=ON L75 AND L76 AND L77 AND L78
L84
               D AU L80 1-3
            13 SEA ABB=ON PLU=ON (L79 OR L80 OR L81 OR L82 OR L83 OR L84)
L85
             1 SEA ABB=ON PLU=ON L22 AND (L74 OR L75 OR L76 OR L77 OR L78)
L86
     FILE 'REGISTRY' ENTERED AT 14:24:28 ON 16 APR 2008
     FILE 'CAPLUS' ENTERED AT 14:24:31 ON 16 APR 2008
                D STAT OUE L85
                D IBIB ABS L85 1-13
     FILE 'MEDLINE, EMBASE, BIOSIS, WPIX' ENTERED AT 14:25:22 ON 16 APR 2008
L87
             14 SEA ABB=ON PLU=ON L85
     FILE 'CAPLUS, WPIX' ENTERED AT 14:25:36 ON 16 APR 2008
             15 DUP REM L85 L87 (12 DUPLICATES REMOVED)
L88
                     ANSWERS '1-13' FROM FILE CAPLUS
```

ANSWERS '14-15' FROM FILE WPIX

D IALL L88 14-15

FILE 'REGISTRY' ENTERED AT 14:25:56 ON 16 APR 2008

FILE 'CAPLUS' ENTERED AT 14:25:59 ON 16 APR 2008
D STAT QUE L18

FILE 'BEILSTEIN' ENTERED AT 14:26:07 ON 16 APR 2008

D STAT QUE L20

FILE 'MARPAT' ENTERED AT 14:26:24 ON 16 APR 2008 D STAT OUE L62

D STAT QUE L62 D STAT QUE L72

L89 36 SEA ABB=ON PLU=ON L62 OR L72

FILE 'CAPLUS' ENTERED AT 14:27:17 ON 16 APR 2008
D IBIB ABS HITSTR L18 TOT

FILE 'MARPAT' ENTERED AT 14:27:20 ON 16 APR 2008

D IBIB ABS QHIT L89 1-36

FILE HOME

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 15 APR 2008 HIGHEST RN 1015083-77-8 DICTIONARY FILE UPDATES: 15 APR 2008 HIGHEST RN 1015083-77-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

FILE CAPLUS

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 16 Apr 2008 VOL 148 ISS 16 FILE LAST UPDATED: 15 Apr 2008 (20080415/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

FILE BEILSTEIN
FILE LAST UPDATED ON April 1, 2008

FILE COVERS 1771 TO 2008.
FILE CONTAINS 10.322,808 SUBSTANCES

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For mo detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

\* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST.

\* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE

\* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE \*

\* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.

\* FOR PRICE INFORMATION SEE HELP COST

>>> Price change as of January 1st, 2008: Connect Time and Structure Search fees re-introduced. See NEWS and HELP COST <<<

FILE MARPAT

FILE CONTENT: 1961-PRESENT VOL 148 ISS 14 (20080411/ED)

SOME MARPAT RECORDS ARE DERIVED FROM INPI DATA FOR 1961-1987

MOST RECENT CITATIONS FOR PATENTS FROM MAJOR ISSUING AGENCIES (COVERAGE TO THESE DATES IS NOT COMPLETE):

US 20080051413 28 FEB 2008
DE 102006039038 21 FEB 2008
EP 1889831 20 FEB 2008
JP 2008044933 28 FEB 2008
WO 2008028336 13 MAR 2008
GB 2440819 13 FEB 2008
FR 2904973 22 FEB 2008
RU 2317993 27 FEB 2008
CA 2593150 06 JAN 2008

Expanded G-group definition display now available.

Effective December 15th the iteration and answer limits in MARPAT have increased from 100,000 to 200,000 for both on-line and batch searches. For more information on MARPAT search limits, type HELP SLIMITS at an arrow prompt.

### FILE MEDLINE

FILE LAST UPDATED: 15 Apr 2008 (20080415/UP). FILE COVERS 1949 TO DATE.

MEDLINE has been updated with the National Library of Medicine's revised 2008 MeSH terms. See HELP RLOAD for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

See HELP RANGE before carrying out any RANGE search.

### FILE EMBASE

FILE COVERS 1974 TO 16 Apr 2008 (20080416/ED)

EMBASE was reloaded on March 30, 2008.

EMBASE is now updated daily. SDI frequency remains weekly (default) and biweekly.

This file contains CAS Registry Numbers for easy and accurate substance identification.

Beginning January 2008, Elsevier will no longer provide EMTREE codes as part of the EMTREE thesaurus in EMBASE. Please update your current-awareness alerts (SDIs) if they contain EMTREE codes.

For further assistance, please contact your local helpdesk.

### FILE BIOSIS

FILE COVERS 1926 TO DATE.

CAS REGISTRY NUMBERS AND CHEMICAL NAMES (CNs) PRESENT FROM JANUARY 1926 TO DATE.

RECORDS LAST ADDED: 9 April 2008 (20080409/ED)

BIOSIS has been augmented with 1.8 million archival records from 1926 through 1968. These records have been re-indexed to match current BIOSIS indexing.

FILE WPIX

FILE LAST UPDATED: 12 APR 2008 <20080412/UP>
MOST RECENT THOMSON SCIENTIFIC UPDATE: 200824 <200824/DW>
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

>>> IPC Reform backfile reclassification has been loaded to the end of
November 2007. No update date (UP) has been created for the
reclassified documents, but they can be identified by
20060101/UPIC and 20061231/UPIC, 20070601/UPIC, 20071001/UPIC and
20071130/UPIC. <<<</pre>

FOR A COPY OF THE DERWENT WORLD PATENTS INDEX STN USER GUIDE, PLEASE VISIT:

http://www.stn-international.de/training\_center/patents/stn\_guide.pdf

FOR DETAILS OF THE PATENTS COVERED IN CURRENT UPDATES, SEE http://scientific.thomson.com/support/patents/coverage/latestupdates/

EXPLORE DERWENT WORLD PATENTS INDEX IN STN ANAVIST, VERSION 2.0:

http://www.stn-international.com/archive/presentations/DWPIAnaVist2\_0710.p

- >>> XML document distribution format now available See HELP XMLDOC <<<
- >>> ECLA Codes and Current US National Classifications have been added see NEWS and HELP CHANGE <<<
- >>> HELP for European Patent Classifications see HELP ECLA, HELP ICO <<<
- >>> Updated PDF files in the following links:
   http://www.stn-international.de/stndatabases/details/ico\_0803.zip
   http://www.stn-international.de/stndatabases/details/epc\_0803.zip
   Supplement of all changed ECLA items:
   http://www.stn-international.de/stndatabases/details/ecla\_0803s.zip <</pre>

=>